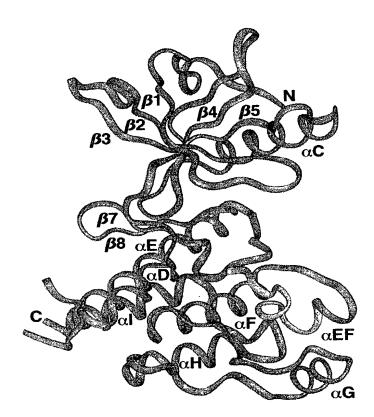
# FG. 1a

		1/67		13,1
-	863 509 1025 856 622	923 568 1083 916 681	953 586 1095 946 741	10:10 605 1114 1004 800
1	F-R2 806 MDPDELPLDEHCERLPYDASKWEFPRDRLKLGKPLGRGAFGQVEADAFGIDKTATCR R1 456MLAGVSEYELP-EDPRWELPRDRLVLGKPLGEGCFGQVLAEAIGLDKDKPNRVT 978VFPCSVYVPDEWEVSREKITLLRELGQGSFGMVEGNARDIIKGEAET F-R1 799 MDPDEVPLDEQCERLPYDASKWEFARERLKLGKSLGRGAFGKVQASAFGIKKSPTCR FRα 576DPMQLPYD-SRWEFPRDGLVLGRVLGSGAFGKVEGTAYGLSRSQPVM	F-R2 864 TVAVKMLKEGATHSEHRALMSELKILIHIGHHLNVVNLLGACTKPGGPLMVIVEFCKFGNR1 510 KVAVKMLKSDATEKDLSDLISEMEMMKMIGKHKNIINLLGACT-QDGPLYVIVEYASKGN 1026 RVAVKTVNESASLRERIEFLNEASVMKGFTCH-HVVRLLGVVSK-GQPTLVVMEL MAHGD F-R1 857 TVAVKMLKEGATASEYKALMTELKILTHIGHHLNVVNLLGACTKQGGPLMVIVEYCKYGN FRα 623 KVAVKMLKFTARSSEKQALMSELKIMTHLGPHLNIVNLLGACTK-SGPIYIITEYCFYGD	F - R2 924 LSTYLRSKRNEFVPYKTKGARFRQGKDYVG	F-R2 954AIPVDLKRRLDSITSSQSSASSGFVEEKSLSDVEEEEAPEDLYKDFLTLEHLICYSFR1 587PSHNPEEQLSSKDLVSCAY 1096ENNPGRPPTLQEMIQMAA F-R1 947PGLEQGKKPRLDSVTSSESFASSGFQEDKSLSDVEEEEDSDGFYKEPITMEDLISYSFFRQ 742 YVPMLERKEVSKYSDIQRSLYDRPASYKK-KSMLDSEVKNLLSDDNSEGLTLLDLLSFTY
	>>	УН — У ПОД — У ОН ЖОО	>H - > - > - > - > - > - > - > - > - > -	>

# FIG. 1b

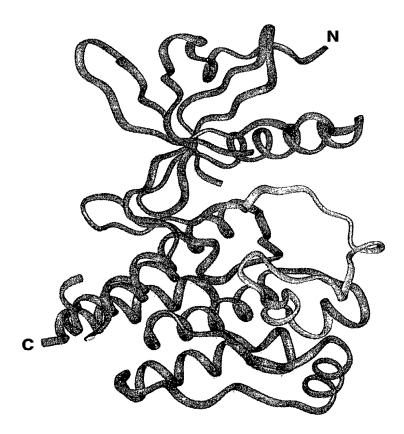
		2/67	
	1070	923	1171
	665	568	765
	1174	1083	1274
	1064	916	1165
	860	681	961
catalytic loop 87 88 activation loop	VEGF-R2 1011 QVAKGMEFDLASRKCIHRDLAARNILLSEKNVVKICÖFGLARDIYKDPDYVRKGDARLPLK	VEGF-R2 1071 WMAPETIFDRVYTIQSDVWSFGVLLWEIFSLGASPYPGVKIDEEFCRRLKEGTRMRRAPDY	VEGF-R2 1131 TTPEMYQTMLDCWHGEPSQRPTFSELVEHLGNLLQANAQQD
	FGFR1 606 QVARGMEYSLASKKCIHRDLAARNVLVTEDNVMKIADFGLARDIHHIDYYKKTTNGRLPVK	FGFR1 666 WMAPEALFDRIYTHQSDVWSFGVLLWEIFTLGGSPYPGVPVEELF-KLLKEGHRMDRKPSN	FGFR1 725 CTNELYMMMRDCWHAVPSQRPTFKQLVEDLDRIVALTSNQE
	IRK 1115 EIADGMEY-LNAKKFVHRDLAARNCMVAHDFTVKIGDFGMTRDIYETDYYRKGGKGLLPVR	IRK 1175 WMAPESLKDGVFTTSSDMWSFGVV WEITSLAEQPYQGLSNEQVL-KFVMDGGYLDLQPDN	IRK 1234 CPERVTDLMRMCWQFNPNMRPTFLEIVNLLKDDLHPSFPEV
	VEGF-R1 1005 QVARGMEFDLSSRKCIHRDLAARNILLSENNVVKIDDFGLARDIYKNPDYVRKGDTRLPLK	VEGF-R1 1065 WMAPESIFDKIYSTKSDVWSYGVLLWEIFSLGGSPYPGVQMDEDFCSRLREGMRMRRAPEY	VEGF-R1 1125 STPEIYQIMLDCWHRDPKERPRFAELVEKLGDLLQANVQQD
	PDGFRα 801 QVARGMEF-LASKKCIHRDLAARNVLLAQGKIVKIDDFGLARDIMHDSNYVSKGSTFLPVK	PDGFRα 861 WMAPESIFDNLYTTLSDVWSYGILLWEIFSLGGTPYPGMMVDSTFYNKIKSGYRMAFKPDH	PDGFRα 921 ATSEVYEIMVKCWNSEPEKRPSFYHLSEIVENLLPGQYKKS

## FIG. 2a



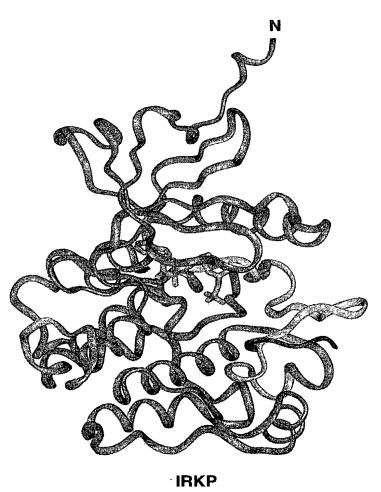
VEGFR2D50P

FIG. 2b

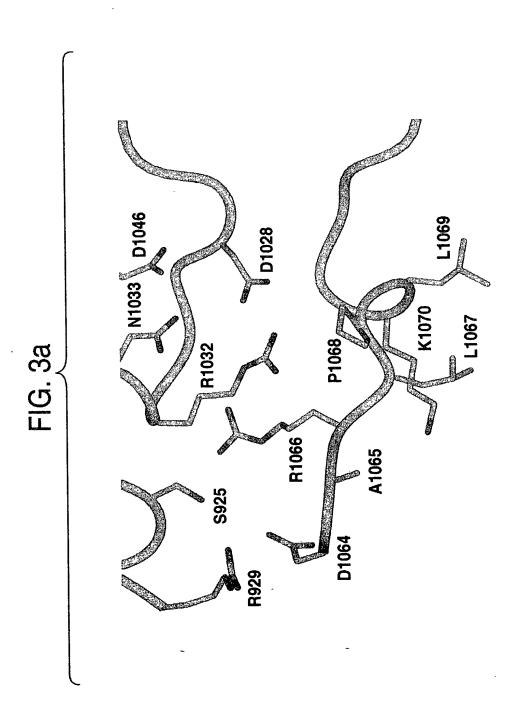


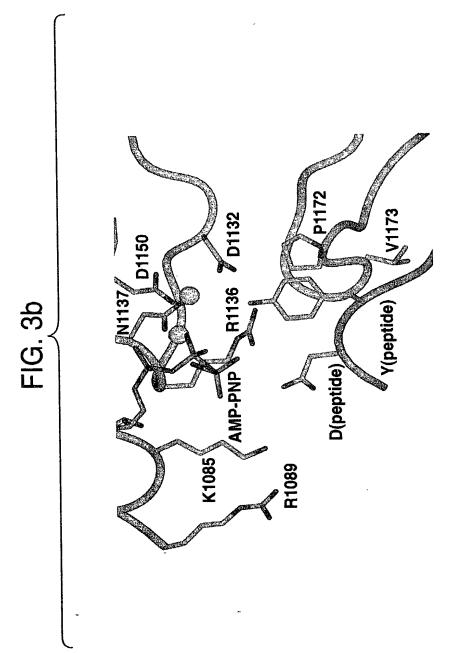
FGFR1

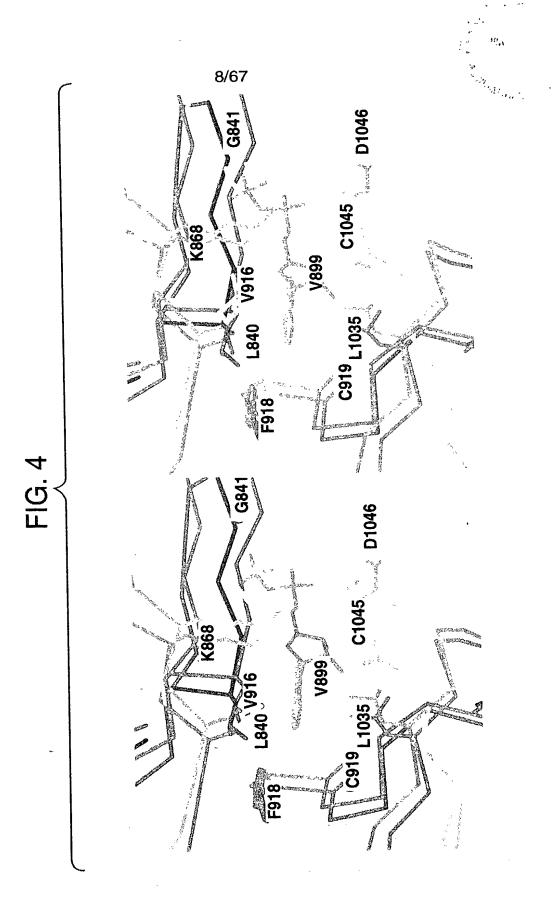
FIG. 2c

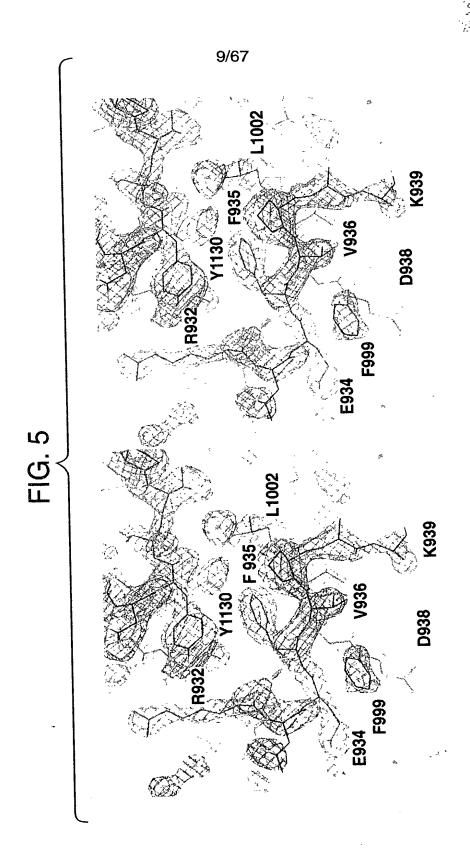


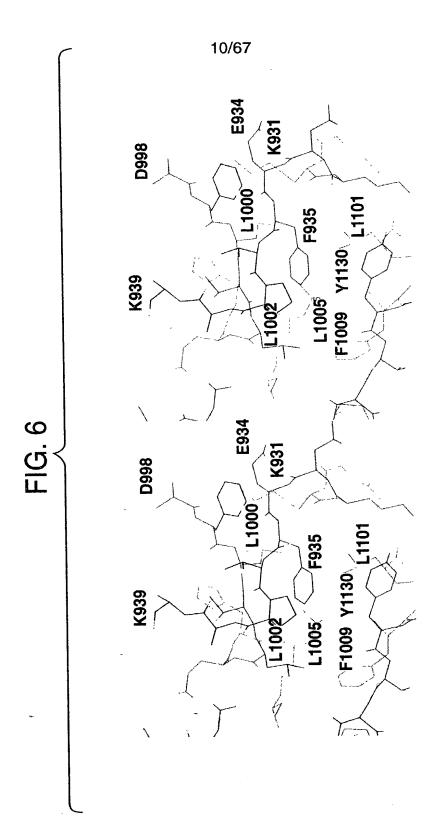












## FIG. 7(1)

		4.5
ATOM	1 CB LEU 820	49.908 45.905 17.938 1.00 48.95
<b>ATOM</b>	2 CG LEU 820	50.568 45.069 16.833 1.00 43.57
<b>ATOM</b>	3 CD1 LEU 820	50.004 45.358 15.456 1.00 43.59
<b>ATOM</b>	4 CD2 LEU 820	52.066 45.345 16.886 1.00 47.45
<b>ATOM</b>	5 C LEU 820	49.216 48.321 17.530 1.00 48.14
<b>ATOM</b>	6 O LEU 820	48.196 48.587 18.187 1.00 52.58
<b>ATOM</b>	9 N LEU 820	50.481 47.725 19.581 1.00 53.68
<b>ATOM</b>	11 CA LEU 820	50.302 47.387 18.117 1.00 50.63
<b>ATOM</b>	12 N PRO 821	49.435 48.842 16.306 1.00 41.32
<b>ATOM</b>	13 CD PRO 821	50.680 48.870 15.520 1.00 45.54
<b>ATOM</b>	14 CA PRO 821	48.465 49.733 15.700 1.00 31.06
<b>ATOM</b>	15 CB PRO 821	49.067 49.985 14.352 1.00 28.89
ATOM	16 CG PRO 821	50.509 50.148 14.734 1.00 43.44
<b>ATOM</b>	17 C PRO 821	47.123 49.165 15.569 1.00 26.14
<b>ATOM</b>	18 O PRO 821	46.948 47.970 15.374 1.00 26.03
ATOM	19 N TYR 822	46.154 50.024 15.776 1.00 16.25
ATOM	21 CA TYR 822	44.799 49.643 15.582 1.00 18.88
ATOM	22 CB TYR 822	44.061 49.519 16.916 1.00 17.42
ATOM	23 CG TYR 822	42.584 49.316 16.728 1.00 18.46
<b>ATOM</b>	24 CD1 TYR 822	41.674 50.341 17.047 1.00 21.12
ATOM	25 CE1 TYR 822	40.314 50.206 16.812 1.00 13.80
ATOM	26 CD2 TYR 822	42.086 48.144 16.175 1.00 12.24
ATOM	27 CE2 TYR 822	40.714 47.997 15.951 1.00 13.44
ATOM	28 CZ TYR 822	39.838 49.028 16.268 1.00 14.38
<b>ATOM</b>	29 OH TYR 822	38.480 48.887 16.073 1.00 19.73
ATOM	31 C TYR 822	44.253 50.760 14.705 1.00 16.93
ATOM	32 O TYR 822	44.172 51.904 15.112 1.00 20.70
ATOM	33 N ASP 823	44.054 50.456 13.439 1.00 15.20
ATOM	35 CA ASP 823	43.509 51.418 12.506 1.00 13.55
ATOM	36 CB ASP 823	43.856 50.945 11.091 1.00 11.37
ATOM	37 CG ASP 823	43.456 51.933 10.016 1.00 16.45
ATOM	38 OD1 ASP 823	42.546 52.754 10.258 1.00 21.86
ATOM	39 OD2 ASP 823	44.022 51.854 8.904 1.00 12.33
ATOM	40 C ASP 823	41.983 51.489 12.738 1.00 14.14
ATOM	41 O ASP 823	41.224 50.722 12.172 1.00 19.73
ATOM	42 N ALA 824	41.539 52.415 13.572 1.00 11.88
ATOM	44 CA ALA 824	40.126 52.554 13.876 1.00 14.80
ATOM	45 CB ALA 824	39.928 53.610 14.973 1.00 12.02
ATOM	46 C ALA 824	39.259 52.893 12.658 1.00 19.09
<b>ATOM</b>	47 O ALA 824	38.062 52.610 12.641 1.00 23.54

### FIG. 7(2)

**ATOM** 48 N SER 825 39.857 53.496 11.635 1.00 18.25 **ATOM** 50 CA SER 825 39.118 53.867 10.450 1.00 12.65 **ATOM** 51 CB SER 825 40,023 54,678 9.543 1.00 11.88 **ATOM** 52 OG SER 825 39.315 55.003 8.370 1.00 20.94 38.669 52.594 9.746 1.00 12.30 **ATOM** 54 C SER 825 **ATOM** 55 O SER 825 37.543 52.461 9.317 1.00 14.94 56 N LYS 826 39.557 51.633 9.642 1.00 14.98 **ATOM** 58 CA LYS 826 39.188 50.396 8.988 1.00 22.45 **ATOM** 59 CB LYS 826 40.445 49.660 8.483 1.00 16.46 **ATOM** 60 CG LYS 826 40.091 48.370 7.820 1.00 23.00 **ATOM ATOM** 61 CD LYS 826 40.962 48.071 6.657 1.00 26.19 62 CE LYS 826 42.391 48.041 7.092 1.00 35.70 **ATOM** 43.272 48.003 5.891 1.00 40.17 **ATOM** 63 NZ LYS 826 67 C LYS 826 38.324 49.437 9.839 1.00 21.47 **ATOM** 68 O LYS 826 37.363 48.850 9.336 1.00 22.56 **ATOM** 38.589 49.376 11.144 1.00 20.96 **ATOM** 69 N TRP 827 71 CA TRP 827 37.917 48.406 11.996 1.00 16.87 **ATOM** 72 CB TRP 827 38.974 47.620 12.785 1.00 18.53 **ATOM ATOM** 73 CG TRP 827 39.942 46.898 11.910 1.00 12.95 39.643 45.810 11.029 1.00 9.73 **ATOM** 74 CD2 TRP 827 75 CE2 TRP 827 40.795 45.562 10.274 1.00 9.36 **ATOM** 38.505 45.038 10.801 1.00 11.54 **ATOM** 76 CE3 TRP 827 77 CD1 TRP 827 41.233 47.231 11.684 1.00 12.87 **ATOM ATOM** 78 NE1 TRP 827 41.753 46.440 10.689 1.00 10.49 40.848 44.565 9.299 1.00 12.36 80 CZ2 TRP 827 **ATOM** 38.556 44.053 9.826 1.00 10.55 **ATOM** 81 CZ3 TRP 827 39.718 43.830 9.087 1.00 11.88 **ATOM** 82 CH2 TRP 827 83 C TRP 827 36.830 48.795 12.953 1.00 17.75 **ATOM ATOM** 35.985 47.951 13.271 1.00 15.08 84 O TRP 827 85 N GLU 828 36,855 50.043 13.416 1.00 16.92 **ATOM** 35.908 50.518 14.413 1.00 19.52 **ATOM** 87 CA GLU 828 88 CB GLU 828 36.289 51.920 14.885 1.00 17.10 **ATOM** 89 CG GLU 828 35.581 52.363 16.148 1.00 12.70 **ATOM ATOM** 90 CD GLU 828 36.106 51.707 17.400 1.00 21.57 37.219 51.118 17.386 1.00 21.15 **ATOM** 91 OE1 GLU 828 92 OE2 GLU 828 35.402 51.819 18.426 1.00 22.43 **ATOM ATOM** 93 C GLU 828 34.494 50.510 13.910 1.00 20.94 34.245 51.024 12.818 1.00 26.92 94 O GLU 828 **ATOM ATOM** 95 N PHE 829 33.569 49.990 14.734 1.00 21.12 97 CA PHE 829 32.138 49.880 14.391 1.00 17.93 **ATOM** 31.791 48.400 14.160 1.00 16.42 **ATOM** 98 CB PHE 829 99 CG PHE 829 30.384 48.164 13.669 1.00 20.17 **ATOM** 

## FIG. 7(3)

30.020 48.484 12.363 1.00 21.31 **ATOM** 100 CD1 PHE 829 29.415 47.612 14.516 1.00 23.04 101 CD2 PHE 829 **ATOM** 28.712 48.254 11.921 1.00 18.76 102 CE1 PHE 829 **ATOM** 28.093 47.375 14.071 1.00 15.20 103 CE2 PHE 829 **ATOM** 104 CZ PHE 829 27.750 47.692 12.792 1.00 17.17 **ATOM** 31.310 50.495 15.533 1.00 14.65 105 C PHE 829 **ATOM** 106 O PHE 829 31.574 50.211 16.686 1.00 16.15 **ATOM** 30,270 51,298 15,224 1,00 13,29 107 N PRO 830 ATOM 29.707 51.633 13.901 1.00 11.63 108 CD PRO 830 **ATOM** 29.481 51.918 16.292 1.00 14.76 **ATOM** 109 CA PRO 830 28.636 52.948 15.565 1.00 13.82 110 CB PRO 830 **ATOM** 28.414 52.364 14.252 1.00 14.42 **ATOM** 111 CG PRO 830 28.629 51.005 17.098 1.00 19.79 112 C PRO 830 **ATOM** 27.750 50.339 16.562 1.00 26.60 **ATOM** 113 O PRO 830 114 N ARG 831 28.830 51.060 18.410 1.00 18.39 **ATOM** 28.085 50.246 19.335 1.00 14.56 116 CA ARG 831 **ATOM** 117 CB ARG 831 28.469 50.580 20.743 1.00 11.53 **ATOM** 29.808 50.050 21.092 1.00 12.65 118 CG ARG 831 **ATOM** 30.117 50.265 22.554 1.00 12.46 **ATOM** 119 CD ARG 831 31.261 51.148 22.584 1.00 20.55 120 NE ARG 831 **ATOM** 32.469 50.756 22.885 1.00 12.04 **ATOM** 122 CZ ARG 831 32.688 49.518 23.234 1.00 23.80 123 NH1 ARG 831 **ATOM** 33.467 51.501 22.526 1.00 23.84 126 NH2 ARG 831 **ATOM** 129 C ARG 831 26.625 50.415 19.174 1.00 18.55 **ATOM** 25.852 49.561 19.607 1.00 25.61 130 O ARG 831 **ATOM** 26.221 51.517 18.552 1.00 25.32 131 N ASP 832 **ATOM** 133 CA ASP 832 24.794 51.734 18.354 1.00 29.47 **ATOM** 24.393 53.230 18.408 1.00 34.15 **ATOM** 134 CB ASP 832 24.817 54.036 17.174 1.00 33.50 135 CG ASP 832 **ATOM** 25.519 53.528 16.280 1.00 34.09 **ATOM** 136 OD1 ASP 832 24.422 55.216 17.110 1.00 41.48 **ATOM** 137 OD2 ASP 832 24.230 51.000 17.139 1.00 27.13 **ATOM** 138 C ASP 832 23.023 50.905 16.991 1.00 28.08 139 O ASP 832 **ATOM** 25.104 50.466 16.290 1.00 24.18 **ATOM** 140 N ARG 833 142 CA ARG 833 24.684 49.695 15.134 1.00 19.93 **ATOM** 25.661 49.902 14.011 1.00 25.94 **ATOM** 143 CB ARG 833 25.313 51.073 13.158 1.00 38.97 **ATOM** 144 CG ARG 833 25.929 50.901 11.766 1.00 53.19 **ATOM** 145 CD ARG 833 25.525 51.930 10.807 1.00 63.47 **ATOM** 146 NE ARG 833 148 CZ ARG 833 25.419 53.229 11.087 1.00.70.42 **ATOM** 25.040 54.080 10.139 1.00 74.08 **ATOM** 149 NH1 ARG 833 25.695 53.690 12.306 1.00 72.08 **ATOM** 152 NH2 ARG 833 24.656 48.218 15.498 1.00 18.62 **ATOM** 155 C ARG 833

FIG. 7(4)

ATOM 156 O ARG 833 24.289 47.370 14.690 1.00 18.27 157 N LEU 834 25.013 47.943 16.747 1.00 18.35 **ATOM** 159 CA LEU 834 25.089 46.600 17.329 1.00 22.59 **ATOM** 26.488 46.398 17.946 1.00 25.91 160 CB LEU 834 **ATOM** ATOM 161 CG LEU 834 27.073 45.003 18.139 1.00 24.64 27.185 44.327 16.805 1.00 21.77 162 CD1 LEU 834 ATOM ATOM 163 CD2 LEU 834 28.428 45.085 18.785 1.00 17.43 164 C LEU 834 23.988 46.326 18.387 1.00 24.77 **ATOM** ATOM 165 O LEU 834 23.886 46.973 19.433 1.00 24.03 ATOM 166 N LYS 835 23.173 45.335 18.087 1.00 28.94 22.072 44.942 18.940 1.00 32.84 ATOM 168 CA LYS 835 **ATOM** 169 CB LYS 835 20.794 44.913 18.081 1.00 31.34 19.529 44.697 18.839 1.00 36.63 **ATOM** 170 CG LYS 835 171 CD LYS 835 18.359 44.407 17.940 1.00 39.31 **ATOM** 172 CE LYS 835 17.074 44.414 18.783 1.00 48.99 **ATOM** 173 NZ LYS 835 17.074 43.448 19.950 1.00 48.86 **ATOM** 177 C LYS 835 22.431 43.532 19.420 1.00 31.79 **ATOM** 178 O LYS 835 22.408 42.609 18.616 1.00 34.57 **ATOM** 179 N LEU 836 22.854 43.395 20.680 1.00 33.17 **ATOM** 181 CA LEU 836 23.229 42.101 21.277 1.00 34.01 **ATOM** ATOM 182 CB LEU 836 23.970 42.292 22.593 1.00 33.96 25.400 42.796 22.462 1.00 42.50 183 CG LEU 836 **ATOM** 26.082 42.858 23.854 1.00 41.15 **ATOM** 184 CD1 LEU 836 **ATOM** 185 CD2 LEU 836 26.153 41.860 21.501 1.00 40.93 22.053 41.181 21.547 1.00 33.27 ATOM 186 C LEU 836 21.017 41.631 22.025 1.00 31.15 187 O LEU 836 **ATOM ATOM** 188 N GLY 837 22.268 39.882 21.330 1.00 36.34 190 CA GLY 837 21.228 38.881 21.536 1.00 34.95 **ATOM** 191 C GLY 837 21.603 37.761 22.497 1.00 35.64 **ATOM** 22.203 37.980 23.554 1.00 39.23 **ATOM** 192 O GLY 837 21.254 36.541 22.126 1.00 35.31 193 N LYS 838 **ATOM** 21.531 35.375 22.962 1.00 37.86 ATOM 195 CA LYS 838 20.647 34.192 22.539 1.00 41.52 196 CB LYS 838 **ATOM** 22.991 34.935 22.989 1.00 35.93 **ATOM** 197 C LYS 838 23.650 34.851 21.946 1.00 34.37 23.499 34.608 24.187 1.00 33.68 22.820 34.757 25.486 1.00 34.48 24.880 34.158 24.363 1.00 37.11 24.927 33.750 25.833 1.00 37.46 23.970 34.710 26.472 1.00 37.04 25.148 32.963 23.474 1.00 39.09 24.303 32.085 23.327 1.00 38.13 26.261 33.013 22.767 1.00 43.08 198 O LYS 838 **ATOM** ATOM 199 N PRO 839 **ATOM** 200 CD PRO 839 ATOM 201 CA PRO 839 202 CB PRO 839 **ATOM** ATOM 203 CG PRO 839 **ATOM** 204 C PRO 839 ATOM 205 O PRO 839 206 N LEU 840 **ATOM** 26.261 33.013 22.767 1.00 43.08

## FIG. 7(5)

208 CA LEU 840 26.646 31.915 21.917 1.00 47:73 **ATOM** 27.396 32.426 20.692 1.00 41.83 209 CB LEU 840 **ATOM** 210 CG LEU 840 26.386 32.957 19.697 1.00 39.60 **ATOM** 27.080 33.697 18.595 1.00 42.69 211 CD1 LEU 840 **ATOM** 25.582 31.795 19.156 1.00 38.40 **ATOM** 212 CD2 LEU 840 27.523 30.987 22.747 1.00 54.84 213 C LEU 840 **ATOM** 27.479 29.768 22.577 1.00 59.76 214 O LEU 840 **ATOM** 215 N GLY 841 28.248 31.563 23.706 1.00 60.51 **ATOM** 29.140 30.781 24.547 1.00 60.96 217 CA GLY 841 **ATOM** 29,660 31.544 25.750 1.00 63.95 218 C GLY 841 **ATOM** 29.497 32.764 25.857 1.00 64.35 219 O GLY 841 **ATOM** 220 N ARG 842 30.279 30.809 26.668 1.00 65.26 **ATOM** 30.823 31.388 27.887 1.00 65.12 222 CA ARG 842 **ATOM** 223 CB ARG 842 30.027 30.897 29.091 1.00 61.50 **ATOM** 32,300 30,995 28,004 1.00 64.23 ATOM 224 C ARG 842 225 O ARG 842 32.957 30.720 26.986 1.00 68.80 **ATOM** 32.822 31.003 29.226 1.00 60.14 **ATOM** 226 N GLY 843 34.206 30.639 29.453 1.00 60.53 228 CA GLY 843 **ATOM** 34.676 31.165 30.789 1.00 62.56 **ATOM** 229 C GLY 843 33.902 31.764 31.535 1.00 61.31 230 O GLY 843 **ATOM** 35.925 30.888 31.140 1.00 66.30 231 N ALA 844 **ATOM** 36.450 31.390 32.403 1.00 69.69 233 CA ALA 844 **ATOM** 37.655 30.574 32.851 1.00 68.47 234 CB ALA 844 **ATOM** 36.839 32.855 32.212 1.00 73.15 235 C ALA 844 **ATOM** 236 O ALA 844 36.723 33.667 33.144 1.00 75.00 **ATOM** 37.251 33.184 30.981 1.00 76.12 237 N PHE 845 **ATOM** 37.699 34.538 30.618 1.00 74.99 **ATOM** 239 CA PHE 845 39.135 34.479 30.014 1.00 72.01 240 CB PHE 845 **ATOM** 36.766 35.353 29.700 1.00 73.81 **ATOM** 241 C PHE 845 36.404 36.499 30.020 1.00 76.82 242 O PHE 845 **ATOM** 36.368 34.767 28.576 1.00 68.48 243 N GLY 846 **ATOM** 35.527 35.495 27.645 1.00 61.76 245 CA GLY 846 **ATOM** 34.102 35.023 27.606 1.00 57.98 246 C GLY 846 **ATOM** 247 O GLY 846 33.658 34.305 28.491 1.00 59.43 **ATOM** 33.400 35.413 26.553 1.00 55.08 248 N GLN 847 **ATOM** 32.006 35.050 26.354 1.00 52.26 250 CA GLN 847 **ATOM** 31.160 35.668 27.449 1.00 55.14 251 CB GLN 847 **ATOM** 29.706 35.703 27.075 1.00 61.40 252 CG GLN 847 **ATOM** 253 CD GLN 847 28.951 36.735 27.844 1.00 65.75 **ATOM** 27.772 36.543 28.150 1.00 69.74 ATOM 254 OE1 GLN 847 29.614 37.852 28.166 1.00 68.83 255 NE2 GLN 847 **ATOM** 31.508 35.573 25.001 1.00 47.29 ATOM 258 C GLN 847 31,637 36,764 24,713 1.00 52.89 259 O GLN 847 **ATOM** 

## FIG. 7(6)

30.912 34.707 24.195 1.00 38.17 ATOM 260 N VAL 848 30.418 35.122 22.898 1.00 30.28 262 CA VAL 848 **ATOM** 30.792 34.137 21.833 1.00 28.01 **ATOM** 263 CB VAL 848 30.542 34.744 20.442 1.00 23.32 264 CG1 VAL 848 **ATOM** 32,239 33,759 22,016 1.00 22,18 265 CG2 VAL 848 **ATOM** 28.920 35.262 22.939 1.00 31.80 266 C VAL 848 **ATOM** 28.221 34.525 23.625 1.00 32.87 ATOM 267 O VAL 848 268 N ILE 849 28.410 36.196 22.166 1.00 29.87 ATOM 26.990 36.436 22.159 1.00 25.35 **ATOM** 270 CA ILE 849 26.602 37.448 23.328 1.00 31.46 271 CB ILE 849 **ATOM** 27.766 38.373 23.732 1.00 32.09 ATOM 272 CG2 ILE 849 25.353 38.244 23.003 1.00 31.00 273 CG1 ILE 849 ATOM 24.895 39.035 24.199 1.00 37.56 274 CD1 ILE 849 **ATOM** 26.493 36.851 20.798 1.00 23.02 **ATOM** 275 C ILE 849 27.167 37.540 20.070 1.00 27.56 276 O ILE 849 **ATOM** 25.376 36.294 20.390 1.00 25.56 277 N GLU 850 **ATOM** 24.802 36.626 19.107 1.00 26.63 279 CA GLU 850 **ATOM** 23.577 35.785 18.894 1.00 27.45 280 CB GLU 850 **ATOM** 23.414 35.361 17.487 1.00 34.57 281 CG GLU 850 **ATOM** 22,155 34,590 17,293 1.00 34,46 282 CD GLU 850 **ATOM** 21.602 34.655 16.184 1.00 42.38 283 OE1 GLU 850 **ATOM** 284 OE2 GLU 850 21.710 33.924 18.248 1.00 40.93 **ATOM** 24.422 38.111 19.028 1.00 27.83 285 C GLU 850 **ATOM** 24.240 38.755 20.047 1.00 25.02 ATOM 286 O GLU 850 24.291 38.640 17.814 1.00 29.11 287 N ALA 851 **ATOM** 23.958 40.043 17.621 1.00 27.32 ATOM 289 CA ALA 851 25.080 40.922 18.170 1.00 18.65 290 CB ALA 851 **ATOM** 291 C ALA 851 23.731 40.387 16.160 1.00 26.61 **ATOM** 24.328 39.785 15.283 1.00 26.99 292 O ALA 851 **ATOM** 22.836 41.343 15.917 1.00 30.82 293 N ASP 852 **ATOM** 22.538 41.862 14.566 1.00 31.76 **ATOM** 295 CA ASP 852 21.050 42.186 14.386 1.00 39.33 296 CB ASP 852 **ATOM** 20.222 40.993 13.993 1.00 47.41 297 CG ASP 852 **ATOM** 19.687 40.330 14.906 1.00 54.12 298 OD1 ASP 852 **ATOM** 20.066 40.754 12.775 1.00 53.02 299 OD2 ASP 852 **ATOM** 23.265 43.204 14.506 1.00 25.97 300 C ASP 852 **ATOM** 23.096 44.021 15.416 1.00 21.64 301 O ASP 852 **ATOM** 24.099 43.411 13.495 1.00 20.18 **ATOM** 302 N ALA 853 24.818 44.672 13.342 1.00 23.55 304 CA ALA 853 **ATOM** 26.305 44.440 13.292 1.00 23.32 305 CB AŁA 853 **ATOM** 24.311 45.222 12.026 1.00 23.89 306 C ALA 853 **ATOM** 24.079 44.439 11.108 1.00 26.15 307 O ALA 853 **ATOM** 24.044 46.526 11.936 1.00 22.87 308 N PHE 854 **ATOM** 

## FIG. 7(7)

310 CA PHE 854 23.529 47.059 10.680 1.00 16.46 ATOM 22.487 48.135 10.901 1.00 23.71 311 CB PHE 854 **ATOM** 22.020 48.758 9.643 1.00 27.62 312 CG PHE 854 **ATOM** 22.476 50.011 9.266 1.00 28.26 313 CD1 PHE 854 **ATOM** 21.205 48.052 8.771 1.00 31.56 314 CD2 PHE 854 **ATOM** 22.136 50.549 8.025 1.00 30.16 315 CE1 PHE 854 **ATOM** 20.856 48.592 7.512 1.00 34.04 316 CE2 PHE 854 **ATOM** 21.328 49.838 7.145 1.00 28.32 317 CZ PHE 854 **ATOM** 24.618 47.569 9.794 1.00 14.10 318 C PHE 854 **ATOM** 25.493 48.299 10.209 1.00 17.34 319 O PHE 854 **ATOM** 24.556 47.163 8.553 1.00 17.45 24.556 47.103 6.555 11.00 18.50 25.559 47.571 7.604 1.00 18.50 47.318 8.020 1.00 22.65 **ATOM** 320 N GLY 855 **ATOM** 322 CA GLY 855 **ATOM** 323 C GLY 855 27.806 48.193 7.777 1.00 26.82 324 O GLY 855 **ATOM** 27.332 46.150 8.580 1.00 23.51 28.740 45.886 8.983 1.00 24.11 **ATOM** 325 N ILE 856 327 CA ILE 856 **ATOM ATOM** 328 CB ILE 856 28.868 44.692 9.980 1.00 27.72 28.535 43.370 9.259 1.00 29.88 329 CG2 ILE 856 **ATOM** 28.535 43.370 9.259 1.00 29.88 30.282 44.663 10.608 1.00 23.26 330 CG1 ILE 856 **ATOM** 30.371 44.079 12.034 1.00 21.70 331 CD1 ILE 856 **ATOM** 29.704 45.665 7.805 1.00 24.83 332 C ILE 856 **ATOM** 30.918 45.721 /.950 1.00 20.2. 29.145 45.460 6.626 1.00 27.69 29.926 45.248 5.420 1.00 31.23 30.918 45.721 7.950 1.00 28.37 333 O ILE 856 **ATOM** 334 N ASP 857 **ATOM ATOM** 336 CA ASP 857 29.566 43.891 4.838 1.00 34.80 337 CB ASP 857 **ATOM** 28.074 43.658 4.811 1.00 40.03 338 CG ASP 857 **ATOM** 28.074 43.658 4.811 1.00 40.03 27.328 44.597 4.448 1.00 43.33 339 OD1 ASP 857 **ATOM** 340 OD2 ASP 857 27.641 42.549 5.200 1.00 46.87 **ATOM** 29.654 46.323 4.370 1.00 32.81 341 C ASP 857 **ATOM** 342 O ASP 857 29.721 46.040 3.183 1.00 38.59 **ATOM** 343 N LYS 858 29.299 47.529 4.813 1.00 34.74 **ATOM** 28.987 48.690 3.946 1.00 34.64 345 CA LYS 858 **ATOM** 30.061 48.947 2.889 1.00 31.38 346 CB LYS 858 **ATOM** 31.462 48.964 3.418 1.00 34.36 347 CG LYS 858 **ATOM** 31.605 49.890 4.603 1.00 39.41 348 CD LYS 858 **ATOM** 33.005 49.791 5.228 1.00 39.87 **ATOM** 349 CE LYS 858 34.059 50.089 4.218 1.00 39.89 350 NZ LYS 858 **ATOM** 27.629 48.709 3.254 1.00 32.27 27.249 49.737 2.724 1.00 35.02 26.891 47.607 3.258 1.00 32.20 25.597 47.610 2.600 1.00 30.11 25.355 46.332 1.785 1.00 30.38 25.365 45.187 2.641 1.00 32.29 354 C LYS 858 **ATOM** 355 O~LYS 858 **ATOM** ATOM 356 N THR 859 358 CA THR 859 **ATOM** ATOM 359 CB THR 859 25.365 45.187 2.641 1.00 32.29 ATOM 360 OG1 THR 859

## FIG. 7(8)

ATOM 362 CG2 THR 859 26.437 46.179 0.757 1.00 32.22 24.450 47.839 3.546 1.00 28.71 **ATOM** 363 C THR 859 24.577 47.647 4.750 1.00 30.55 364 O THR 859 **ATOM** 23.303 48.201 2.989 1.00 30.07 365 N ALA 860 **ATOM** 22.123 48.474 3.784 1.00 28.01 367 CA ALA 860 **ATOM** 21.141 49.253 2.928 1.00 23.78 368 CB ALA 860 **ATOM** 21.461 47.222 4.394 1.00 28.00 ATOM 369 C ALA 860 370 O ALA 860 20.251 47.100 4.373 1.00 31.77 **ATOM** 22.228 46.325 5.008 1.00 29.99 371 N THR 861 **ATOM** 21.663 45.078 5.577 1.00 27.77 373 CA THR 861 **ATOM** 22.186 43.857 4.808 1.00 20.97 374 CB THR 861 **ATOM** 23.614 43.926 4.687 1.00 27.23 **ATOM** 375 OG1 THR 861 21.608 43.794 3.449 1.00 29.39 **ATOM** 377 CG2 THR 861 21.986 44.790 7.055 1.00 31.89 378 C THR 861 **ATOM** 379 O THR 861 23.095 45.077 7.532 1.00 34.73 **ATOM** 21.037 44.183 7.770 1.00 34.09 380 N CYS 862 **ATOM** 21.250 43.805 9.178 1.00 31.63 **ATOM** 382 CA CYS 862 19.922 43.756 9.943 1.00 27.50 383 CB CYS 862 **ATOM** 384 SG CYS 862 19.863 44.908 11.327 1.00 41.79 **ATOM** 21.876 42.424 9.146 1.00 25.51 385 C CYS 862 **ATOM** 386 O CYS 862 21.241 41.492 8.700 1.00 30.38 **ATOM** 387 N ARG 863 23.136 42.307 9.541 1.00 27.68 **ATOM** 23.839 41.025 9.532 1.00 28.29 389 CA ARG 863 **ATOM** 25.211 41.210 8.882 1.00 36.18 **ATOM** 390 CB ARG 863 25.775 39.945 8.275 1.00 48.71 391 CG ARG 863 **ATOM** 27.282 40.034 7.943 1.00 58.46 392 CD ARG 863 **ATOM** 27.824 38.721 7.550 1.00 65.04 393 NE ARG 863 **ATOM** 29.112 38.452 7.330 1.00 65.66 ATOM 395 CZ ARG 863 29.482 37.219 6.985 1.00 67.60 396 NH1 ARG 863 **ATOM** 30.030 39.409 7.421 1.00 66.49 399 NH2 ARG 863 **ATOM** 24.006 40.409 10.943 1.00 28.34 **ATOM** 402 C ARG 863 ATOM 403 O ARG 863 24.337 41.125 11.904 1.00 24.64 23,735 39,100 11.078 1.00 23.23 404 N THR 864 **ATOM** 23.900 38.426 12.364 1.00 18.91 ATOM 406 CA THR 864 23.062 37.099 12.489 1.00 19.40 ATOM 407 CB THR 864 21.672 37.435 12.547 1.00 24.20 ATOM 408 OG1 THR 864 23.371 36.351 13.793 1.00 8.83 ATOM 410 CG2 THR 864 25.385 38.148 12.462 1.00 20.93 ATOM 411 C THR 864 ATOM 412 O THR 864 26.001 37.736 11.468 1.00 20.14 25.962 38.442 13.634 1.00 16.03 ATOM 413 N VAL 865 ATOM 415 CA VAL 865 27.381 38.254 13.897 1.00 16.69 28.175 39.620 13.906 1.00 17.70 ATOM 416 CB VAL 865 28.107 40.299 12.539 1.00 21.22 ATOM 417 CG1 VAL 865

## FIG. 7(9)

27.625 40.554 14.979 1.00 20.92 418 CG2 VAL 865 **ATOM** 27.533 37.660 15.276 1.00 15.90 419 C VAL 865 **ATOM** 26.552 37.554 15.995 1.00 16.43 420 O VAL 865 **ATOM** 28.775 37.295 15.612 1.00 16.37 **ATOM** 421 N ALA 866 29.210 36.753 16.910 1.00 18.08 **ATOM** 423 CA ALA 866 30.022 35.490 16.691 1.00 7.41 424 CB ALA 866 **ATOM** 425 C ALA 866 30.117 37.834 17.588 1.00 23.87 **ATOM** 31.121 38.261 16.998 1.00 24.17 426 O ALA 866 **ATOM** 427 N VAL 867 29.790 38.235 18.827 1.00 26.69 **ATOM** 30.534 39.268 19.554 1.00 20.37 429 CA VAL 867 **ATOM** 430 CB VAL 867 29.592 40.365 20.088 1.00 17.71 **ATOM** 30.361 41.586 20.519 1.00 9.32 431 CG1 VAL 867 **ATOM** 28.635 40.753 19.027 1.00 14.57 432 CG2 VAL 867 **ATOM** 31.320 38.748 20.728 1.00 21.67 **ATOM** 433 C VAL 867 30.784 38.085 21.606 1.00 23.57 434 O VAL 867 **ATOM** 32.616 38.982 20.694 1.00 21.65 **ATOM** 435 N LYS 868 33.471 38.593 21.782 1.00 27.02 437 CA LYS 868 **ATOM** 34.860 38.169 21.289 1.00 29.71 438 CB LYS 868 **ATOM** 34.842 36.963 20.405 1.00 37.08 439 CG LYS 868 **ATOM** 36.151 36.810 19.666 1.00 44.81 440 CD LYS 868 **ATOM** 441 CE LYS 868 36.183 35.512 18.868 1.00 45.52 **ATOM** 37.548 35.298 18.274 1.00 47.28 442 NZ LYS 868 **ATOM** 33.585 39.842 22.647 1.00 26.11 **ATOM** 446 C LYS 868 33.962 40.914 22.188 1.00 24.72 447 O LYS 868 **ATOM** 33.184 39.721 23.888 1.00 29.77 **ATOM** 448 N MET 869 33.299 40.821 24.803 1.00 32.95 450 CA MET 869 **ATOM** 31.958 41.491 24.996 1.00 30.57 **ATOM** 451 CB MET 869 30.900 40.542 25.463 1.00 32.29 **ATOM** 452 CG MET 869 29.348 41.157 24.961 1.00 42.68 453 SD MET 869 **ATOM** 29.251 42.663 25.919 1.00 35.32 **ATOM** 454 CE MET 869 455 C MET 869 33.778 40.205 26.095 1.00 40.29 **ATOM** 33.921 38.967 26.216 1.00 35.26 456 O MET 869 **ATOM** 34.079 41.066 27.051 1.00 46.88 457 N LEU 870 **ATOM** 34.521 40.576 28.337 1.00 51.36 459 CA LEU 870 **ATOM** 35.544 41.549 28.937 1.00 48.55 **ATOM** 460 CB LEU 870 36.862 41.677 28.180 1.00 44.32 **ATOM** 461 CG LEU 870 37.734 42.739 28.855 1.00 36.89 462 CD1 LEU 870 **ATOM** 37.535 40.306 28.149 1.00 41.04 **ATOM** 463 CD2 LEU 870 33.344 40.306 29.311 1.00 53.63 464 C LEU 870 **ATOM** 32.163 40.615 29.037 1.00 52.68 465 O LEU 870 **ATOM** 33.675 39.644 30.412 1.00 56.89 466 N LYS 871 **ATOM** 32.695 39.346 31.426 1.00 58.53 468 CA LYS 871 **ATOM** 33.083 38.077 32.169 1.00 59.89 469 CB LYS 871 **ATOM** 

## FIG. 7(10)

470 CG LYS 871 31,903 37,220 32.546 1.00 63.81 **ATOM ATOM** 471 CD LYS 871 31.912 35.965 31.719 1.00 65.43 33,268 35,318 31.853 1.00 70.59 **ATOM** 472 CE LYS 871 33.318 34.051 31.135 1.00 76.57 **ATOM** 473 NZ LYS 871 477 C LYS 871 32.649 40.518 32.404 1.00 59.44 **ATOM** 478 O LYS 871 33.582 41.342 32.464 1.00 56.75 **ATOM ATOM** 479 N GLU 872 31.566 40.571 33.177 1.00 61.50 481 CA GLU 872 31.357 41.618 34.177 1.00 64.12 **ATOM** 482 CB GLU 872 29.928 41.539 34.739 1.00 66.85 **ATOM** 28.846 41.903 33.729 1.00 71.27 483 CG GLU 872 **ATOM** 484 CD GLU 872 29.060 41.218 32.387 1.00 74.41 **ATOM** 28.900 39.980 32.326 1.00 76.27 485 OE1 GLU 872 **ATOM** 29.443 41.903 31.411 1.00 74.20 486 OE2 GLU 872 **ATOM** 487 C GLU 872 32.387 41.424 35.288 1.00 60.87 **ATOM** 488 O GLU 872 32.331 40.441 36.026 1.00 61.34 **ATOM** 489 N GLY 873 33.368 42.319 35.335 1.00 57.40 **ATOM** 34,408 42,223 36,337 1.00 53,93 **ATOM** 491 CA GLY 873 492 C GLY 873 35.703 41.641 35.803 1.00 52.30 **ATOM** 36.518 41.103 36.563 1.00 51.95 **ATOM** 493 O GLY 873 494 N ALA 874 35.881 41.721 34.491 1.00 51.13 **ATOM** 37.090 41.217 33.862 1.00 51.21 **ATOM** 496 CA ALA 874 497 CB ALA 874 36.875 41.049 32.335 1.00 48.57 **ATOM** 498 C ALA 874 38.270 42.172 34.199 1.00 50.40 **ATOM** 499 O ALA 874 38.101 43.388 34.369 1.00 48.57 **ATOM ATOM** 500 N THR 875 39.465 41.609 34.245 1.00 48.33 40.657 42.334 34.617 1.00 51.59 502 CA THR 875 **ATOM ATOM** 503 CB THR 875 41.572 41.428 35.447 1.00 54.42 42.677 42.184 35.937 1.00 60.69 504 OG1 THR 875 **ATOM** 506 CG2 THR 875 **ATOM** 42.107 40.280 34.593 1.00 60.52 507 C THR 875 **ATOM** 41.455 42.830 33.448 1.00 51.15 41.395 42.263 32.372 1.00 52.26 **ATOM** 508 O THR 875 509 N HIS 876 42.343 43.770 33.733 1.00 53.93 **ATOM** 43.215 44.392 32.737 1.00 55.68 **ATOM** 511 CA HIS 876 44.170 45.383 33.419 1.00 54.06 512 CB HIS 876 **ATOM ATOM** 513 CG HIS 876 45,609 44,980 33,361 1.00 56,52 46.595 45.314 32.487 1.00 56.83 514 CD2 HIS 876 **ATOM** 515 ND1 HIS 876 46.191 44.149 34.297 1.00 60.22 **ATOM** 47.472 43.992 34.009 1.00 62.12 **ATOM** 517 CE1 HIS 876 518 NE2 HIS 876 47.739 44.689 32.916 1.00 59.66 **ATOM** 44.003 43.385 31.898 1.00 54.72 **ATOM** 520 C HIS 876 521 O HIS 876 44.510 43.712 30.810 1.00 54.08 **ATOM** 44.167 42.189 32.434 1.00 52.07 **ATOM** 522 N SER 877 **ATOM** 524 CA SER 877 44.872 41.160 31.704 1.00 53.73

## FIG. 7(11)

45.622 40.256 32.669 1.00 57.58 ATOM 525 CB SER 877 46.559 41.054 33.379 1.00 63.62 **ATOM** 526 OG SER 877 43.880 40.410 30.810 1.00 51.29 **ATOM** 528 C SER 877 44.227 39.962 29.715 1.00 50.11 529 O SER 877 **ATOM** 42.629 40.320 31.246 1.00 47.72 530 N GLU 878 **ATOM** 41.620 39.696 30.410 1.00 45.39 532 CA GLU 878 **ATOM** 40.335 39.483 31.201 1.00 48.19 533 CB GLU 878 **ATOM** 40.383 38.191 32.013 1.00 60.86 534 CG GLU 878 **ATOM ATOM** 535 CD GLU 878 39.304 38.086 33.092 1.00 68.27 38.448 37.162 33.027 1.00 70.85 536 OE1 GLU 878 **ATOM** 39.336 38.911 34.029 1.00 67.92 **ATOM** 537 OE2 GLU 878 538 C GLU 878 41.448 40.702 29.277 1.00 40.09 **ATOM** 539 O GLU 878 41.536 40.365 28.104 1.00 38.92 **ATOM** 41.393 41.966 29.659 1.00 34.60 **ATOM** 540 N HIS 879 542 CA HIS 879 41,252 43.072 28.732 1.00 36.68 **ATOM** 41.070 44.392 29.505 1.00 44.03 **ATOM** 543 CB HIS 879 40.637 45.547 28.652 1.00 43.54 544 CG HIS 879 ATOM 39.403 46.025 28.364 1.00 40.08 **ATOM** 545 CD2 HIS 879 546 ND1 HIS 879 41.529 46.307 27.917 1.00 39.08 **ATOM** 40.860 47.192 27.202 1.00 40.82 **ATOM** 548 CE1 HIS 879 39.572 47.045 27.452 1.00 49.01 549 NE2 HIS 879 **ATOM** 42.455 43.172 27.797 1.00 34.17 551 C HIS 879 **ATOM** 42.293 43.494 26.626 1.00 33.65 552 O HIS 879 **ATOM** 43.664 42.993 28.319 1.00 33.25 **ATOM** 553 N ARG 880 44.838 43.033 27.470 1.00 29.84 **ATOM** 555 CA ARG 880 46,124 42,932 28,299 1.00 36,53 **ATOM** 556 CB ARG 880 46.615 41.470 28.452 1.00 50.57 **ATOM 557 CG ARG** 880 48.121 41.276 28.649 1.00 56.95 **ATOM** 558 CD ARG 880 48.555 41.748 29.960 1.00 63.99 **ATOM** 559 NE ARG 880 49.030 42.967 30.175 1.00 66.67 561 CZ ARG 880 **ATOM ATOM** 562 NH1 ARG 880 49.391 43.327 31.397 1.00 66.45 49.170 43.813 29.157 1.00 66.52 565 NH2 ARG 880 **ATOM** 568 C ARG 880 44.741 41.799 26.533 1.00 29.72 **ATOM** 45,246 41.808 25.401 1.00 21.81 **ATOM** 569 O ARG 880 44,070 40.747 27.006 1.00 28.49 570 N ALA 881 **ATOM** 43.942 39.514 26.227 1.00 31.72 572 CA ALA 881 **ATOM** 43.587 38.342 27.142 1.00 31.57 573 CB ALA 881 **ATOM** 42.978 39.592 25.044 1.00 29.98 **ATOM** 574 C ALA 881 575 O ALA 881 43.319 39.154 23.944 1.00 31.95 **ATOM** 41.766 40.099 25.273 1.00 27.12 576 N LEU 882 **ATOM** 40.804 40.248 24.193 1.00 27.43 578 CA LEU 882 **ATOM** 40.804 40.248 24.193 1.00 27.43 39.493 40.784 24.728 1.00 23.93 579 CB LEU 882 **ATOM** 38.402 40.925 23.662 1.00 25.91 580 CG LEU 882 **ATOM** 

#### FIG. 7(12)

581 CD1 LEU 882 38.435 39.722 22.743 1.00 21.9121 **ATOM** 37.013 41.102 24.325 1.00 23.61 **ATOM** 582 CD2 LEU 882 41.368 41.230 23.151 1.00 30.62 583 C LEU 882 **ATOM** 584 O LEU 882 41.312 40.982 21.945 1.00 27.61 **ATOM** 41.940 42.325 23.643 1.00 29.74 **ATOM** 585 N MET 883 42.548 43.364 22.808 1.00 30.75 587 CA MET 883 **ATOM** 43.001 44.516 23.738 1.00 27.47 588 CB MET 883 **ATOM** 43.432 45.828 23.084 1.00 33.64 589 CG MET 883 **ATOM** 590 SD MET 883 42.313 46.592 21.882 1.00 33.18 **ATOM** 41.031 47.285 22.943 1.00 33.54 591 CE MET 883 **ATOM** 43.711 42.756 21.965 1.00 29.92 592 C MET 883 **ATOM** 43.862 43.022 20.766 1.00 28.38 593 O MET 883 **ATOM** 44.501 41.893 22.588 1.00 29.75 594 N SER 884 **ATOM** 45.597 41.231 21.912 1.00 28.29 596 CA SER 884 **ATOM** 597 CB SER 884 46.343 40.391 22.923 1.00 32.03 **ATOM** 47.220 39.502 22.270 1.00 44.59 **ATOM** 598 OG SER 884 45.091 40.329 20.778 1.00 29.39 600 C SER 884 **ATOM** 45.595 40.359 19.654 1.00 28.92 **ATOM** 601 O SER 884 602 N GLU 885 44.084 39.526 21.071 1.00 25.33 **ATOM** 43.559 38.661 20.058 1.00 27.47 **ATOM** 604 CA GLU 885 42.563 37.692 20.661 1.00 31.61 **ATOM** 605 CB GLU 885 41.142 38.108 20.642 1.00 46.01 **ATOM** 606 CG GLU 885 40.215 36.903 20.799 1.00 55.19 **ATOM** 607 CD GLU 885 40.018 36.469 21.964 1.00 58.80 **ATOM** 608 OE1 GLU 885 39.715 36.379 19.762 1.00 54.01 609 OE2 GLU 885 **ATOM ATOM** 610 C GLU 885 42.945 39.470 18.924 1.00 28.59 42.833 38.983 17.805 1.00 26.67 611 O GLU 885 **ATOM** 42.560 40.712 19.211 1.00 27.06 612 N LEU 886 **ATOM** 41.994 41.594 18.205 1.00 23.75 614 CA LEU 886 **ATOM** 41.483 42.887 18.847 1.00 22.79 615 CB LEU 886 **ATOM** 41.122 44.033 17.905 1.00 17.60 616 CG LEU 886 **ATOM** 39.981 43.608 16.999 1.00 11.98 617 CD1 LEU 886 **ATOM** 40.747 45.285 18.702 1.00 18.31 **ATOM** 618 CD2 LEU 886 619 C LEU 886 43.049 41.936 17.147 1.00 24.77 **ATOM** 42.767 41.880 15.939 1.00 22.15 **ATOM** 620 O LEU 886 44.265 42.246 17.602 1.00 25.08 621 N LYS 887 **ATOM** 45.384 42.613 16.722 1.00 24.94 623 CA LYS 887 **ATOM** 46.517 43.227 17.544 1.00 29.70 624 CB LYS 887 **ATOM** 625 CG LYS 887 46.105 44.304 18.560 1.00 30.67 **ATOM** 45.556 45.551 17.895 1.00 28.99 626 CD LYS 887 **ATOM** 45.170 46.645 18.923 1.00 26.07 627 CE LYS 887 **ATOM** 46.354 47.216 19.621 1.00 17.59 628 NZ LYS 887 **ATOM** 45.921 41.407 15.925 1.00 25.59 632 C LYS 887 **ATOM** 

### FIG. 7(13)

ATOM 633 O LYS 887 46.388 41.547 14.793 1.00 30.23 634 N ILE 888 45.917 40.235 16.542 1.00 20.48 **ATOM ATOM** 636 CA ILE 888 46.347 39.028 15.859 1.00 21.46 637 CB ILE 888 46.306 37.795 16.816 1.00 22.73 **ATOM** 46.604 36.556 16.047 1.00 24.05 **ATOM** 638 CG2 ILE 888 47.355 37.929 17.937 1.00 23.32 **ATOM** 639 CG1 ILE 888 47.092 37.058 19.190 1.00 18.29 640 CD1 ILE 888 **ATOM** ATOM 641 C ILE 888 45.392 38.822 14.663 1.00 19.51 45.834 38.710 13.529 1.00 19.15 642 O ILE 888 **ATOM** 44.088 38.828 14.922 1.00 15.54 **ATOM** 643 N LEU 889 43.078 38.677 13.872 1.00 20.73 645 CA LEU 889 **ATOM** 41.658 38.818 14.446 1.00 19.41 **ATOM** 646 CB LEU 889 647 CG LEU 889 41.204 37.652 15.372 1.00 22.61 **ATOM** 39.735 37.752 15.697 1.00 13.49 **ATOM** 648 CD1 LEU 889 649 CD2 LEU 889 41.500 36.263 14.764 1.00 18.87 **ATOM** ATOM 650 C LEU 889 43.308 39.678 12.762 1.00 24.12 651 O LEU 889 43.342 39.344 11.584 1.00 28.65 **ATOM** 43.461 40.931 13.138 1.00 29.62 652 N ILE 890 **ATOM** 43.753 41.953 12.158 1.00 26.41 **ATOM** 654 CA ILE 890 43.966 43.310 12.865 1.00 24.45 **ATOM** 655 CB ILE 890 44.555 44.333 11.888 1.00 30.36 **ATOM** 656 CG2 ILE 890 42.645 43.825 13.438 1.00 19.80 657 CG1 ILE 890 **ATOM** 42.812 45.061 14.241 1.00 14.93 ATOM 658 CD1 ILE 890 45.053 41.519 11.415 1.00 28.37 **ATOM** 659 C ILE 890 **ATOM** 660 O ILE 890 45.126 41.553 10.191 1.00 24.83 46.066 41.099 12.164 1.00 27.37 661 N HIS 891 **ATOM** 47.309 40.659 11.567 1.00 27.76 ATOM 663 CA HIS 891 48.277 40.175 12.654 1.00 36.80 664 CB HIS 891 **ATOM** 49.509 39.507 12.100 1.00 47.58 665 CG HIS 891 **ATOM** 50.811 39.869 12.147 1.00 46.38 666 CD2 HIS 891 **ATOM** 49.450 38.394 11.276 1.00 52.71 667 ND1 HIS 891 **ATOM** 50.660 38.114 10.825 1.00 50.46 **ATOM** 669 CE1 HIS 891 51.505 38.993 11.340 1.00 54.62 670 NE2 HIS 891 **ATOM ATOM** 672 C HIS 891 47.098 39.536 10.537 1.00 27.01 47.522 39.647 9.402 1.00 32.82 **ATOM** 673 O HIS 891 674 N ILE 892 46.580 38.403 10.995 1.00 24.99 **ATOM** 46.300 37.216 10.181 1.00 23.19 45.233 36.282 10.907 1.00 24.73 44.643 35.295 9.941 1.00 20.03 45.828 35.522 12.104 1.00 26.32 47.015 36.222 12.787 1.00 36.72 45.700 37.625 8.848 1.00 22.57 46.115 37.155 7.775 1.00 25.20 676 CA ILE 892 **ATOM** 677 CB ILE 892 **ATOM ATOM** 678 CG2 ILE 892 679 CG1 ILE 892 **ATOM** 680 CD1 ILE 892 **ATOM** 681 C ILE 892 **ATOM** 682 O ILE 892 **ATOM** 

# FIG. 7(14)

<b>ATOM</b>	683 N GLY 893	44.699 38.492	8.916 1.00 23.88
<b>ATOM</b>	685 CA GLY 893	44.034 38.910	7.702 1.00 25.37
<b>ATOM</b>	686 C GLY 893	42.794 38.080	7.403 1.00 25.54
<b>ATOM</b>	687 O GLY 893	42.303 37.326	8.224 1.00 32.60
<b>ATOM</b>	688 N HIS 894	42.327 38.149	6.176 1.00 26.97
<b>ATOM</b>	690 CA HIS 894	41.120 37.457	5.797 1.00 26.35
<b>ATOM</b>	691 CB HIS 894	40.233 38.464	5.042 1.00 31.72
<b>ATOM</b>	692 CG HIS 894	39.114 37.833	4.274 1.00 35.68
<b>ATOM</b>	693 CD2 HIS 894	37.818 37.609	4.608 1.00 34.18
<b>ATOM</b>	694 ND1 HIS 894	39.271 37.346	2.989 1.00 38.36
<b>ATOM</b>	696 CE1 HIS 894	38.121 36.854	2.568 1.00 36.24
<b>ATOM</b>	697 NE2 HIS 894	37.224 37.004	3.527 1.00 35.86
<b>ATOM</b>	699 C HIS 894	41.253 36.182	4.958 1.00 24.38
<b>ATOM</b>	700 O HIS 894	42.045 36.108	4.007 1.00 24.24
ATOM	701 N HIS 895	40.426 35.202	5.280 1.00 17.00
<b>ATOM</b>	703 CA HIS 895	40.379 33.994	4.494 1.00 18.62
<b>ATOM</b>	704 CB HIS 895	41.363 32.929	4.931 1.00 15.85
<b>ATOM</b>	705 CG HIS 895	41.446 31.814	3.943 1.00 21.47
<b>ATOM</b>	706 CD2 HIS 895	42.076 31.737	2.745 1.00 17.93
<b>ATOM</b>	707 ND1 HIS 895	40.675 30.676	4.042 1.00 21.96
<b>ATOM</b>	709 CE1 HIS 895	40.819 29.956	2.938 1.00 21.22
<b>ATOM</b>	710 NE2 HIS 895	41.663 30.578	2.137 1.00 10.16
<b>ATOM</b>	712 C HIS 895	38.979 33.467	4.626 1.00 15.66
<b>ATOM</b>	713 O HIS 895	38.396 33.656	5.663 1.00 18.76
<b>ATOM</b>	714 N LEU 896	38.419 32.865	3.567 1.00 21.74
<b>ATOM</b>	716 CA LEU 896	37.042 32.306	3.584 1.00 18.37
ATOM	717 CB LEU 896	36.652 31.762	2.210 1.00 17.64
<b>ATOM</b>	718 CG LEU 896	35.297 31.068	2.218 1.00 25.15
<b>ATOM</b>	719 CD1 LEU 896	34.218 32.077	2.454 1.00 24.41
<b>ATOM</b>	720 CD2 LEU 896	35.042 30.342	0.934 1.00 25.59
<b>ATOM</b>	721 C LEU 896	36.867 31.172	4.569 1.00 17.58
<b>ATOM</b>	722 O LEU 896	35.783 30.937	5.068 1.00 23.11
<b>ATOM</b>	723 N ASN 897	37.952 30.475	4.849 1.00 15.99
ATOM	725 CA ASN 897	37.878 29.340	5.725 1.00 18.36
<b>ATOM</b>	726 CB ASN 897	38.589 28.134	5.078 1.00 20.86
<b>ATOM</b>	727 CG ASN 897	37.928 27.689	
ATOM	728 OD1 ASN 897	38.567 27.692	2.694 1.00 14.51
ATOM	729 ND2 ASN 897	36.639 27.346	3.799 1.00 12.11
ATOM	732 C ASN 897	38.293 29.541	7.188 1.00 25.65
ATOM	733 O ASN 897	38.648 28.556	7.858 1.00 22.22
ATOM	734 N VAL 898	38.357 30.800	
ATOM	736 CA VAL 898	38.631 31.079	
ATOM	737 CB VAL 898	40.036 31.719	9.457 1.00 11.47

## FIG. 7(15)

738 CG1 VAL 898 41.146 30.813 9.017 1.00 14.76 **ATOM** 739 CG2 VAL 898 40.236 33.119 8.883 1.00 8.71 **ATOM** 37.475 31.959 9.477 1.00 15.57 **ATOM** 740 C VAL 898 **ATOM** 741 O VAL 898 36.698 32.382 8.620 1.00 17.87 37.226 32.049 10.773 1.00 18.55 **ATOM** 742 N VAL 899 744 CA VAL 899 36.155 32.882 11.264 1.00 20.68 **ATOM** 35.757 32.487 12.720 1.00 19.98 **ATOM** 745 CB VAL 899 746 CG1 VAL 899 34.618 33.384 13.202 1.00 18.29 **ATOM ATOM** 747 CG2 VAL 899 35.346 31.016 12.788 1.00 12.67 36.807 34.272 11.244 1.00 21.95 748 C VAL 899 **ATOM** 749 O VAL 899 37.725 34.517 12.003 1.00 21.42 **ATOM** 36.352 35.164 10.363 1.00 23.43 750 N ASN 900 **ATOM** 36.930 36.526 10.226 1.00 23.52 **ATOM** 752 CA ASN 900 36.737 37.061 8.803 1.00 19.45 753 CB ASN 900 **ATOM** 37.350 36.177 7.782 1.00 19.58 **ATOM** 754 CG ASN 900 38.578 36.087 7.667 1.00 17.65 **ATOM** 755 OD1 ASN 900 36.511 35.528 7.004 1.00 20.34 **ATOM** 756 ND2 ASN 900 36.484 37.641 11.152 1.00 17.00 **ATOM** 759 C ASN 900 **ATOM** 760 O ASN 900 35.343 37.704 11.598 1.00 16.94 37.413 38.544 11.384 1.00 17.25 761 N LEU 901 **ATOM** 37.167 39.733 12.160 1.00 17.98 **ATOM** 763 CA LEU 901 764 CB LEU 901 38,494 40.447 12.426 1.00 16.80 **ATOM** 765 CG LEU 901 38.444 41.819 13.101 1.00 14.17 **ATOM** 38.018 41.673 14.560 1.00 11.71 **ATOM** 766 CD1 LEU 901 39.782 42.435 13.008 1.00 2.76 **ATOM** 767 CD2 LEU 901 **ATOM** 768 C LEU 901 36.354 40.578 11.174 1.00 20.28 36.669 40.612 9.965 1.00 18.06 **ATOM** 769 O LEU 901 35.280 41.180 11.686 1.00 19.74 **ATOM** 770 N LEU 902 **ATOM** 772 CA LEU 902 34.398 42.031 10.917 1.00 15.84 773 CB LEU 902 32.950 41.593 11.087 1.00 11.70 **ATOM** 32.615 40.230 10.473 1.00 13.49 **ATOM** 774 CG LEU 902 31.142 39.827 10.774 1.00 13.78 **ATOM** 775 CD1 LEU 902 **ATOM** 776 CD2 LEU 902 32.856 40.270 8.981 1.00 12.15 34.566 43.486 11.345 1.00 19.59 **ATOM** 777 C LEU 902 **ATOM** 778 O LEU 902 34.466 44.380 10.510 1.00 23.95 779 N GLY 903 34.854 43.724 12.625 1.00 20.15 **ATOM** 781 CA GLY 903 35.037 45.090 13.114 1.00 21.60 **ATOM** 35.147 45.075 14.620 1.00 24.02 **ATOM** 782 C GLY 903 783 O GLY 903 35.070 43.991 15.194 1.00 26:53 **ATOM** ATOM -784 N ALA 904 35.305 46.236 15.269 1.00 25.19 35.411 46.293 16.740 1.00 18.80 786 CA ALA 904 **ATOM** 36.830 46.074 17.177 1.00 12.62 787 CB ALA 904 **ATOM ATOM** 788 C ALA 904 34.886 47.559 17.386 1.00 20.83

## FIG. 7(16)

789 O ALA 904 **ATOM** 34.789 48.616 16.765 1.00 26.12 **ATOM** 790 N CYS 905 34.617 47.443 18.674 1.00 21.21 34.128 48.530 19.493 1.00 19.91 **ATOM** 792 CA CYS 905 **ATOM** 793 CB CYS 905 32.804 48.160 20.115 1.00 16.08 794 SG CYS 905 31.561 47.894 18.851 1.00 15.32 **ATOM ATOM** 795 C CYS 905 35.176 48.687 20.556 1.00 23.00 35.245 47.890 21.486 1.00 24.21 796 O CYS 905 **ATOM** 797 N THR 906 36.042 49.674 20.361 1.00 26.02 **ATOM ATOM** 799 CA THR 906 37.140 49.945 21.283 1.00 29.46 800 CB THR 906 38.514 49.768 20.574 1.00 26.67 **ATOM** 801 OG1 THR 906 38.635 50.739 19.526 1.00 29.06 **ATOM** 38.648 48.363 20.001 1.00 23.13 803 CG2 THR 906 **ATOM** 804 C THR 906 37.130 51.346 21.928 1.00 30.07 **ATOM** 805 O THR 906 37.642 51.522 23.036 1.00 29.29 **ATOM** 806 N LYS 907 36.582 52.332 21.228 1.00 32.81 **ATOM** 808 CA LYS 907 36.554 53.686 21.745 1.00 39.38 **ATOM** 35.982 54.637 20.701 1.00 41.03 **ATOM** 809 CB LYS 907 810 CG LYS 907 34.536 54.432 20.386 1.00 48.86 **ATOM ATOM** 811 CD LYS 907 34.071 55.528 19.427 1.00 57.25 33.996 56.878 20.143 1.00 63.62 812 CE LYS 907 **ATOM** 33.688 58.001 19.213 1.00 68.81 **ATOM** 813 NZ LYS 907 35.796 53.779 23.070 1.00 44.43 817 C LYS 907 **ATOM** 35.094 52.867 23.442 1.00 44.52 818 O LYS 907 **ATOM** 819 N PRO 908 36.034 54.838 23.857 1.00 49.18 **ATOM** 37.147 55.794 23.712 1.00 50.93 **ATOM** 820 CD PRO 908 **ATOM** 821 CA PRO 908 35.358 55.022 25.149 1.00 46.86 35.963 56.324 25.647 1.00 49.68 **ATOM** 822 CB PRO 908 **ATOM** 823 CG PRO 908 37.387 56.216 25.143 1.00 51.43 33.852 55.145 25.036 1.00 44.06 824 C PRO 908 **ATOM** 825 O PRO 908 33.345 55.600 24.008 1.00 44.40 **ATOM** 826 N GLY 909 33.154 54.772 26.110 1.00 41.44 **ATOM** 828 CA GLY 909 31.698 54.842 26.135 1.00 37.38 **ATOM ATOM** 829 C GLY 909 30.999 53.502 26.035 1.00 38.26 29.778 53.439 25.751 1.00 40.07 830 O GLY 909 **ATOM** 31.753 52.424 26.264 1.00 36.39 **ATOM** 831 N GLY 910 31.178 51.087 26.190 1.00 34.35 833 CA GLY 910 **ATOM** 32.180 49.961 26.360 1.00 31.85 **ATOM** 834 C GLY 910 835 O GLY 910 33.394 50.235 26.528 1.00 27.95 **ATOM ATOM** 836 N PRO 911 31.710 48.686 26.319 1.00 27.95 30.280 48.339 26.197 1.00 28.51 **ATOM** 837 CD PRO 911 838 CA PRO 911 32.511 47.463 26.467 1.00 25.21 **ATOM** 839 CB PRO 911 31.438 46.393 26.724 1.00 27.44 **ATOM ATOM** 840 CG PRO 911 30.315 46.840 25.891 1.00 22.45

## FIG. 7(17)

ATOM 841 C PRO 911 33.340 47.118 25.234 1.00 22.33 842 O PRO 911 32.903 47.366 24.124 1.00 23.57 **ATOM ATOM** 843 N LEU 912 34.548 46.581 25.430 1.00 22.75 35.412 46.177 24.308 1.00 23.22 ATOM 845 CA LEU 912 ATOM 846 CB LEU 912 36.778 45.685 24.812 1.00 23.67 ATOM 847 CG LEU 912 38.095 45.759 24.005 1.00 24.34 ATOM 848 CD1 LEU 912 38.988 44.618 24.490 1.00 20.11 ATOM 849 CD2 LEU 912 37.906 45.745 22.477 1.00 12.72 ATOM 850 C LEU 912 34.692 45.010 23.627 1.00 22.56 ATOM 851 O LEU 912 34,342 44,029 24,283 1.00 17.69 852 N MET 913 34.417 45.142 22.334 1.00 24.19 **ATOM** ATOM 854 CA MET 913 33.724 44.085 21.617 1.00 21.51 855 CB MET 913 **ATOM** 32.264 44.456 21.429 1.00 22.09 856 CG MET 913 31.489 44.461 22.728 1.00 22.26 **ATOM** 857 SD MET 913 29.829 45.009 22.484 1.00 24.17 **ATOM** ATOM 858 CE MET 913 30.127 46.676 22.205 1.00 20.40 859 C MET 913 34.386 43.768 20.295 1.00 20.42 **ATOM ATOM** 860 O MET 913 34,701 44.657 19.519 1.00 21.08 861 N VAL 914 34,703 42,491 20,102 1,00 23,72 **ATOM** ATOM 863 CA VAL 914 35.354 42.001 18.891 1.00 20.24 36.614 41.170 19.232 1.00 16.92 ATOM 864 CB VAL 914 ATOM 865 CG1 VAL 914 37.254 40.637 17.958 1.00 19.36 37.629 42.055 19.972 1.00 13.30 ATOM 866 CG2 VAL 914 34.296 41.210 18.132 1.00 19.70 ATOM 867 C VAL 914 ATOM 868 O VAL 914 33.836 40.191 18.587 1.00 26.45 869 N ILE 915 33.844 41.775 17.026 1.00 19.86 **ATOM ATOM** 871 CA ILE 915 32.806 41.212 16.179 1.00 20.42 872 CB ILE 915 32.034 42.384 15.455 1.00 18.44 **ATOM** 873 CG2 ILE 915 30.721 41.909 14.869 1.00 12.35 **ATOM** 874 CG1 ILE 915 31.756 43.531 16.426 1.00 17.60 **ATOM** 31,358 44,822 15,735 1.00 15,14 **ATOM** 875 CD1 ILE 915 876 C ILE 915 33.457 40.287 15.115 1.00 23.98 **ATOM** 34.361 40.722 14.373 1.00 23.30 **ATOM** 877 O ILE 915 33.054 39.011 15.075 1.00 20.08 878 N VAL 916 **ATOM** 33.594 38.089 14.077 1.00 17.64 ATOM 880 CA VAL 916 **ATOM** 881 CB VAL 916 34.543 37.003 14.680 1.00 9.09 **ATOM** 882 CG1 VAL 916 35.703 37.685 15.350 1.00 5.05 **ATOM** 883 CG2 VAL 916 33.817 36.126 15.678 1.00 10.26 32,422 37,486 13,342 1.00 17,74 ATOM 884 C VAL 916 **ATOM** 885 O VAL 916 31.275 37.790 13.664 1.00 20.02 32.684 36.702 12.303 1.00 14.74 ATOM 886 N GLU 917 31.589 36.073 11.577 1.00 13.03 32.120 35.409 10.332 1.00 14.06 888 CA GLU 917 **ATOM** 32,120 35,409 10,332 1,00 14,06 ATOM 889 CB GLU 917

## FIG. 7(18)

ATOM 890 CG GLU 917 32.946 36.348 9.464 1.00 24.11 ATOM 891 CD GLU 917 33.543 35.651 8.258 1.00 26.52 33.543 35.651 8.258 1.00 26.52 33.060 35.904 7.139 1.00 27.67 34.480 34.841 8.425 1.00 28.39 **ATOM** 892 OE1 GLU 917 ATOM 893 OE2 GLU 917 

34.480
34.841
8.425
1.00
28.39

30.853
35.051
12.434
1.00
14.78

31.445
34.344
13.234
1.00
14.35

29.557
34.958
12.229
1.00
19.12

28.688
34.042
12.966
1.00
18.07

27.334
34.721
13.168
1.00
18.48

26.275
33.840
13.748
1.00
17.83

26.328
33.456
15.081
1.00
18.65

25.213
33.400
12.953
1.00
21.10

25.336
32.639
15.613
1.00
18.12

24.210
32.580
13.473
1.00
18.12

24.274
32.201
14.799
1.00
17.78

28.487
32.805
12.113
1.00
18.83

28.081
32.917
10.964
1.00
11.61

28.761
31.635
12.676
1.00
19.00

29.855
29.566
12.069
1.00
16.78

 **ATOM** 894 C GLU 917 ATOM 895 O GLU 917 **ATOM** 896 N PHE 918 ATOM 898 CA PHE 918 **ATOM** 899 CB PHE 918 ATOM 900 CG PHE 918 **ATOM** 901 CD1 PHE 918 **ATOM** 902 CD2 PHE 918 **ATOM** 903 CE1 PHE 918 ATOM 904 CE2 PHE 918 ATOM 905 CZ PHE 918 906 C PHE 918 ATOM ATOM 907 O PHE 918 ATOM 908 N CYS 919 **ATOM** 910 CA CYS 919 **ATOM** 911 CB CYS 919 912 SG CYS 919 **ATOM ATOM** 913 C CYS 919 914 O CYS 919 **ATOM** 26.269 29.653 11.818 1.00 18.06 24.998 29.130 12.318 1.00 28.13 23.799 29.581 11.459 1.00 25.17 915 N LYS 920 **ATOM** ATOM 917 CA LYS 920 **ATOM** 918 CB LYS 920 **ATOM** 919 CG LYS 920 23.595 28.799 10.207 1.00 33.78 920 CD LYS 920 **ATOM** 22.658 29.509 9.250 1.00 40.32 21.261 29.706 9.829 1.00 51.94 **ATOM** 921 CE LYS 920 **ATOM** 922 NZ LYS 920 20.343 30.396 8.845 1.00 56.09 **ATOM** 926 C LYS 920 24.813 27.679 12.700 1.00 28.53 24.020 27.405 13.592 1.00 31.57 25.533 26.757 12.078 1.00 24.89 25.328 25.362 12.409 1.00 21.12 25.497 24.518 11.171 1.00 20.75 24.588 24.917 10.084 1.00 22.95 23.224 24.734 10.219 1.00 27.55 927 O LYS 920 **ATOM ATOM** 928 N PHE 921 **ATOM** 930 CA PHE 921 **ATOM** 931 CB PHE 921 **ATOM** 932 CG PHE 921 933 CD1 PHE 921 **ATOM** 25.077 25.564 8.975 1.00 29.40 **ATOM** 934 CD2 PHE 921 **ATOM** 935 CE1 PHE 921 22.362 25.205 9.269 1.00 35.42 24.237 26.041 8.013 1.00 32.24 22.869 25.870 8.154 1.00 38.81 **ATOM** 936 CE2 PHE 921 937 CZ PHE 921 **ATOM** 26.158 24.823 13.535 1.00 21.23 26.002 23.664 13.900 1.00 22.74 938 C PHE 921 **ATOM** 939 O PHE 921 **ATOM** 

## FIG. 7(19)

27.047 25.659 14.065 1.00 18.39 940 N GLY 922 **ATOM** 27.906 25.257 15.172 1.00 17.62 **ATOM** 942 CA GLY 922 29.115 24.455 14.759 1.00 18.42 **ATOM** 943 C GLY 922 29.331 24.230 13.581 1.00 20.81 944 O GLY 922 ATOM 29.903 24.011 15.729 1.00 22.93 945 N ASN 923 **ATOM** 31.092 23.223 15.430 1.00 24.85 947 CA ASN 923 **ATOM** 31.867 22.837 16.705 1.00 29.68 948 CB ASN 923 **ATOM** 31.212 21.710 17.493 1.00 39.14 949 CG ASN 923 **ATOM** 31.252 20.550 17.087 1.00 41.11 950 OD1 ASN 923 ATOM 951 ND2 ASN 923 30.662 22.038 18.660 1.00 35.87 **ATOM** 30.818 22.019 14.523 1.00 21.09 954 C ASN 923 **ATOM** 29.685 21.566 14.370 1.00 20.59 955 O ASN 923 **ATOM** 31.867 21.523 13.896 1.00 21.13 **ATOM** 956 N LEU 924 31.740 20.431 12.957 1.00 22.85 958 CA LEU 924 **ATOM** 33.019 20.377 12.126 1.00 23.67 **ATOM** 959 CB LEU 924 33.019 19.462 10.920 1.00 17.22 960 CG LEU 924 **ATOM** 31.776 19.699 10.125 1.00 18.21 **ATOM** 961 CD1 LEU 924 34.268 19.729 10.095 1.00 23.82 962 CD2 LEU 924 **ATOM** 31.414 19.062 13.558 1.00 22.65 **ATOM** 963 C LEU 924 30.601 18.326 13.013 1.00 26.13 964 O LEU 924 **ATOM** 31.035 18.742 14.687 1.00 20.06 965 N SER 925 **ATOM** 31.853 17.463 15.383 1.00 25.99 967 CA SER 925 **ATOM** 32.741 17.400 16.623 1.00 27.28 968 CB SER 925 **ATOM** 32.426 16.272 17.416 1.00 32.86 **ATOM** 969 OG SER 925 30.432 17.217 15.812 1.00 26.73 971 C SER 925 **ATOM** 29.863 16.148 15.552 1.00 30.93 972 O SER 925 **ATOM** 29.892 18.190 16.534 1.00 24.48 973 N THR 926 **ATOM** 28.535 18.129 16.996 1.00 19.27 975 CA THR 926 ATOM 28.258 19.336 17.901 1.00 16.05 976 CB THR 926 **ATOM** 29.230 19.374 18.951 1.00 18.42 977 OG1 THR 926 **ATOM** 26.927 19.216 18.550 1.00 13.93 979 CG2 THR 926 **ATOM** 27.610 18.048 15.758 1.00 20.47 980 C THR 926 **ATOM** 26.654 17.258 15.711 1.00 25.12 **ATOM** 981 O THR 926 27.961 18.760 14.701 1.00 18.97 982 N TYR 927 **ATOM** 27.128 18.715 13.515 1.00 20.97 **ATOM** 984 CA TYR 927 27.597 19.720 12.464 1.00 18.52 985 CB TYR 927 **ATOM** 26.708 19.683 11.230 1.00 18.69 986 CG TYR 927 **ATOM** 25.391 20.196 11.266 1.00 14.64 987 CD1 TYR 927 **ATOM** 24.567 20.173 10.125 1.00 13.73 988 CE1 TYR 927 **ATOM** 27.173 19.138 10.031 1.00 22.28 989 CD2 TYR 927 **ATOM** 26.347 19.104 8.879 1.00 24.92 **ATOM** 990 CE2 TYR 927 25.058 19.626 8.944 1.00 16.40 991 CZ TYR 927 **ATOM** 24.285 19.600 7.819 1.00 23.87 992 OH TYR 927 **ATOM** 

## FIG. 7(20)

ATOM 994 C TYR 927 27.118 17.343 12.855 1.00 23.85 **ATOM** 995 O TYR 927 26.078 16.860 12.428 1.00 24.11 ATOM 996 N LEU 928 28.313 16.793 12.665 1.00 28.91 **ATOM** 998 CA LEU 928 28.513 15.495 12.020 1.00 31.09 ATOM 999 CB LEU 928 30.017 15.192 11.863 1.00 27.50 ATOM 1000 CG LEU 928 30.813 16.159 10.953 1.00 24.21 ATOM 1001 CD1 LEU 928 32.302 15.880 11.065 1.00 24.38 ATOM 1002 CD2 LEU 928 30.343 16.097 9.514 1.00 12.63 ATOM 1003 C LEU 928 27.801 14.369 12.747 1.00 31.00 ATOM 1004 O LEU 928 27.164 13.540 12.117 1.00 31.53 ATOM 1005 N ARG 929 27.883 14.351 14.067 1.00 34.05 ATOM 1007 CA ARG 929 27.193 13.316 14.833 1.00 40.50 ATOM 1008 CB ARG 929 27.406 13.552 16.325 1.00 41.71 ATOM 1009 CG ARG 929 28.358 12.605 16.969 1.00 40.42 ATOM 1010 CD ARG 929 29.253 13.359 17.908 1.00 49.36 ATOM 1011 NE ARG 929 28.521 13.947 19.020 1.00 62.28 ATOM 1013 CZ ARG 929 28.946 14.985 19.749 1.00 65.86 ATOM 1014 NH1 ARG 929 28.178 15.432 20.753 1.00 66.98 ATOM 1017 NH2 ARG 929 30.122 15.573 19.492 1.00 58.39 ATOM 1020 C ARG 929 25.678 13.304 14.529 1.00 42.76 ATOM 1021 O ARG 929 25.075 12.234 14.370 1.00 44.84 ATOM 1022 N SER 930 25.089 14.498 14.412 1.00 41.42 ATOM 1024 CA SER 930 23.663 14.677 14.150 1.00 37.04 ATOM 1025 CB SER 930 23.324 16.151 14.250 1.00 38.80 ATOM 1026 OG SER 930 23.662 16.816 13.041 1.00 37.58 ATOM 1028 C SER 930 23.226 14.226 12.774 1.00 38.41 ATOM 1029 O SER 930 22.034 14.254 12.451 1.00 43.98 ATOM 1030 N LYS 931 24.179 13.865 11.936 1.00 37.60 ATOM 1032 CA LYS 931 23.845 13.472 10.590 1.00 38.82 ATOM 1033 CB LYS 931 24.575 14.387 9.606 1.00 43.10 ATOM 1034 CG LYS 931 24.388 15.864 9.884 1.00 45.62 ATOM 1035 CD LYS 931 22.999 16.302 9.487 1.00 49.49 ATOM 1036 CE LYS 931 22.901 16.444 7.985 1.00 46.94 ATOM 1037 NZ LYS 931 21.501 16.690 7.568 1.00 49.54 ATOM 1041 C LYS 931 24.136 12.011 10.264 1.00 39.02 ATOM 1042 O LYS 931 23.991 11.615 9.111 1.00 42.79 ATOM 1043 N ARG 932 24.522 11.199 11.247 1.00 37.44 ATOM 1045 CA ARG 932 24.793 9.776 10.971 1.00 38.33 ATOM 1046 CB ARG 932 ATOM 1047 CG ARG 932 26.456 9.461 12.798 1.00 33.92 ATOM 1048 CD ARG 932 26.812 8.729 14.043 1.00 35.88 ATOM 1049 NE ARG 932 28.223 8.929 14.368 1.00 43.26 ATOM 1051 CZ ARG 932 28.720 8.909 15.604 1.00 45.56

## FIG. 7(21)

ATOM 1052 NH1 ARG 932 30.018 9.098 15.809 1.00 47.32 ATOM 1055 NH2 ARG 932 27.916 8.725 16.645 1.00 53.04 ATOM 1058 C ARG 932 23.621 9.087 10.273 1.00 41.54 ATOM 1059 O ARG 932 23.821 8.135 9.532 1.00 41.31 ATOM 1060 N ASN 933 22.412 9.582 10.536 1.00 44.37 ATOM 1062 CA ASN 933 21.181 9.069 9.956 1.00 47.14 ATOM 1063 CB ASN 933 19.974 9.453 10.824 1.00 54.55 ATOM 1064 CG ASN 933 19.783 8.545 12.050 1.00 57.14 ATOM 1065 OD1 ASN 933 20.622 7.693 12.369 1.00 54.11 ATOM 1066 ND2 ASN 933 18.668 8.752 12.757 1.00 57.76 ATOM 1069 C ASN 933 20.974 9.680 8.589 1.00 49.60 ATOM 1070 O ASN 933 20.260 9.125 7.753 1.00 55.62 ATOM 1071 N GLU 934 21.494 10.888 8.403 1.00 52.11 ATOM 1073 CA GLU 934 21.365 11.580 7.122 1.00 52.39 ATOM 1074 CB GLU 934 20.859 13.007 7.323 1.00 56.14 ATOM 1075 CG GLU 934 19.434 13.095 7.822 1.00 59.40 ATOM 1076 CD GLU 934 19.332 13.686 9.211 1.00 63.97 ATOM 1077 OE1 GLU 934 18.427 13.250 9.953 1.00 69.17 ATOM 1078 OE2 GLU 934 20.138 14.580 9.563 1.00 64.27 ATOM 1079 C GLU 934 22.677 11.593 6.332 1.00 50.45 ATOM 1080 O GLU 934 23.188 12.663 5.961 1.00 50.70 ATOM 1081 N PHE 935 23.205 10.396 6.070 1.00 46.25 ATOM 1083 CA PHE 935 24.440 10.225 5.325 1.00 41.20 ATOM 1084 CB PHE 935 25.638 10.121 6.268 1.00 40.97 ATOM 1085 CG PHE 935 26.923 9.800 5.555 1.00 39.81 ATOM 1086 CD1 PHE 935 27.327 8.478 5.378 1.00 34.65 ATOM 1087 CD2 PHE 935 27.676 10.815 4.970 1.00 33.02 ATOM 1088 CE1 PHE 935 28.455 8.180 4.617 1.00 32.30 ATOM 1089 CE2 PHE 935 28.793 10.515 4.218 1.00 29.96 ATOM 1090 CZ PHE 935 29.181 9.201 4.037 1.00 29.08 ATOM 1091 C PHE 935 24.474 9.006 4.412 1.00 40.49 ATOM 1092 O PHE 935 24.394 7.871 4.865 1.00 40.47 ATOM 1093 N VAL 936 24.694 9.237 3.133 1.00 38.66 ATOM 1095 CA VAL 936 24.809 8.138 2.208 1.00 43.29 ATOM 1096 CB VAL 936 23.663 8.113 1.221 1.00 40.39 ATOM 1097 CG1 VAL 936 23.739 9.312 0.280 1.00 34.50 ATOM 1098 CG2 VAL 936 23.720 6.841 0.444 1.00 42.47 ATOM 1099 C VAL 936 26.087 8.436 1.438 1.00 49.63 ATOM 1100 O VAL 936 26.322 9.585 1.081 1.00 55.64 ATOM 1101 N PRO 937 26.960 7.433 1.222 1.00 50.29 ATOM 1102 CD PRO 937 26.966 6.087 1.822 1.00 49.69 ATOM 1103 CA PRO 937 28.207 7.669 0.483 1.00 50.65 ATOM 1104 CB PRO 937 28.676 6.260 0.177 1.00 46.68

#### FIG. 7(22)

28.378 5.582 1.493 1.00 47.42 ATOM 1105 CG PRO 937 28.019 8.501 -0.774 1.00 53.83 ATOM 1106 C PRO 937 ATOM 1107 O PRO 937 28.644 9.558 -0.937 1.00 53.64 27.153 8.046 -1.660 1.00 54.91 ATOM 1108 N TYR 938 26.918 8.803 -2.859 1.00 62.52 ATOM 1110 CA TYR 938 27.580 8.161 -4.080 1.00 67.73 ATOM 1111 CB TYR 938 ATOM 1120 C TYR 938 25,443 8.800 -3.059 1.00 67.31 ATOM 1121 O TYR 938 24,722 8,082 -2.361 1.00 66.13 25,027 9,601 -4.038 1.00 75.30 ATOM 1122 N LYS 939 23.639 9.770 -4.445 1.00 81.21 ATOM 1124 CA LYS 939 23.209 11.254 -4.284 1.00 80.04 ATOM 1125 CB LYS 939 23.543 9.331 -5.921 1.00 87.24 ATOM 1126 C LYS 939 24.582 9.384 -6.646 1.00 90.23 ATOM 1127 O LYS 939 17.986 15.692 3.023 1.00 53.00 ATOM 1129 CB ASP 998 20.489 15.723 3.377 1.00 55.33 ATOM 1130 C ASP 998 21.051 16.058 4.426 1.00 56.29 ATOM 1131 O ASP 998 19.408 16.931 1.400 1.00 54.52 ATOM 1134 N ASP 998 ATOM 1136 CA ASP 998 19.279 16.514 2.829 1.00 55.12 20.900 14.687 2.653 1.00 52.90 ATOM 1137 N PHE 999 ATOM 1139 CA PHE 999 21.984 13.834 3.111 1.00 46.86 21.841 12.420 2.528 1.00 51.05 ATOM 1140 CB PHE 999 20.897 11.537 3.296 1.00 55.62 ATOM 1141 CG PHE 999 21.249 10.236 3.606 1.00 56.12 ATOM 1142 CD1 PHE 999 19.671 12.022 3.751 1.00 60.98 ATOM 1143 CD2 PHE 999 20.397 9.422 4.368 1.00 61.93 ATOM 1144 CE1 PHE 999 18.816 11.222 4.509 1.00 61.09 ATOM 1145 CE2 PHE 999 ATOM 1146 CZ PHE 999 19.183 9.917 4.820 1.00 60.64 23.373 14.302 2.837 1.00 41.06 ATOM 1147 C PHE 999 ATOM 1148 O PHE 999 23.632 14.937 1.820 1.00 36.04 ATOM 1149 N LEU 1000 24.238 14.057 3.812 1.00 37.57 ATOM 1151 CA LEU 1000 25.651 14.326 3.652 1.00 36.08 26.401 14.306 4.985 1.00 35.67 ATOM 1152 CB LEU 1000 25.923 15.286 6.057 1.00 36.23 ATOM 1153 CG LEU 1000 26.941 15.370 7.201 1.00 29.94 ATOM 1154 CD1 LEU 1000 25.707 16.654 5.435 1.00 38.66 ATOM 1155 CD2 LEU 1000 ATOM 1156 C LEU 1000 26.089 13.139 2.756 1.00 35.16 ATOM 1157 O LEU 1000 25.330 -12.167 2.569 1.00 32.68 ATOM 1158 N THR 1001 27.292 13.228 2.201 1.00 29.92 27.803 12.236 1.285 1.00 25.42 ATOM 1160 CA THR 1001 27.396 12.560 -0.178 1.00 30.10 ATOM 1161 CB THR 1001

# FIG. 7(23)

<b>ATOM</b>	1162 OG1 THR 1001	28.055	13.771	-0.605	1.00 33.54
<b>ATOM</b>	1164 CG2 THR 1001	25.878			1.00 29.24
<b>ATOM</b>	1165 C THR 1001	29.303	12.388		1.00 27.68
<b>ATOM</b>	1166 O THR 1001	29.805	13.303		1.00 28.02
<b>ATOM</b>	1167 N LEU 1002	30.020	11.552		1.00 26.85
<b>ATOM</b>	1169 CA LEU 1002	31.454	11.636		1.00 24.39
<b>ATOM</b>	1170 CB LEU 1002	32.044	10.545		1.00 22.71
<b>ATOM</b>	1171 CG LEU 1002	32.269	9.304	0.573	1.00 27.80
<b>ATOM</b>	1172 CD1 LEU 1002	32.727	8.142		1.00 27.11
<b>ATOM</b>	1173 CD2 LEU 1002	33.295	9.592	1.670	1.00 24.64
<b>ATOM</b>	1174 C LEU 1002	31.908	12.995		1.00 26.97
<b>ATOM</b>	1175 O LEU 1002	32.967	13.459	0.506	1.00 26.84
<b>ATOM</b>	1176 N GLU 1003	31.063	13.682		1.00 27.89
<b>ATOM</b>	1178 CA GLU 1003	31.428	15.000	-1.185	1.00 28.02
<b>ATOM</b>	1179 CB GLU 1003	30.419	15.503	-2.208	1.00 32.50
<b>ATOM</b>	1180 CG GLU 1003	30.988	16.624	-3.077	1.00 37.49
<b>ATOM</b>	1181 CD GLU 1003	31.915	16.121	-4.170	1.00 38.89
<b>ATOM</b>	1182 OE1 GLU 1003	33.065	15.743	-3.886	1.00 43.61
<b>ATOM</b>	1183 OE2 GLU 1003	31.488	16.102	-5.331	1.00 46.97
<b>ATOM</b>	1184 C GLU 1003	31.591	16.044	-0.117	1.00 25.24
<b>ATOM</b>	1185 O GLU 1003	32.485	16.885	-0.211	1.00 26.57
<b>ATOM</b>	1186 N HIS 1004	30.748	15.953	0.913	1.00 23.16
<b>ATOM</b>	1188 CA HIS 1004	30.746	16.884	2.040	1.00 19.58
<b>ATOM</b>	1189 CB HIS 1004	29.508	16.719	2.912	1.00 19.12
<b>ATOM</b>	1190 CG HIS 1004	28.227	17.024	2.208	1.00 23.47
<b>ATOM</b>	1191 CD2 HIS 1004	27.173	17.784	2.570	1.00 23.78
<b>ATOM</b>	1192 ND1 HIS 1004	27.911	16.508	0.964	1.00 27.88
<b>ATOM</b>	1194 CE1 HIS 1004	26.718	16.936	0.596	1.00 20.57
<b>ATOM</b>	1195 NE2 HIS 1004	26.246	17.710	1.554	1.00 23.61
<b>ATOM</b>	1197 C HIS 1004	31.940	16.631	2.885	1.00 21.64
ATOM	1198 O HIS 1004	32.753	17.508	3.075	1.00 25.00
<b>ATOM</b>	1199 N LEU 1005	32.055	15.419	3.394	1.00 23.11
<b>ATOM</b>	1201 CA LEU 1005	33.186	15.072	4.222	1.00 23.79
	1202 CB LEU 1005	33.131	13.581	4.589	1.00 24.17
	1203 CG LEU 1005	32.183	13.199	5.743	1.00 27.48
		31.030	14.150	5.821	1.00 25.44
-		31.679	11.771	5.627	1.00 22.50
<b>ATOM</b>	1206 C LEU 1005	34.506	15.467	3.558	1.00 20.41
<b>ATOM</b>					1.00 21.82
ATOM	1208 N ILE 1006	34.668	15.212	2.264	1.00 19.50

## FIG. 7(24)

ATOM 1210 CA ILE 1006 35.914 15.589 1.609 1.00 18.77 ATOM 1211 CB ILE 1006 36.128 14.806 0.276 1.00 16.46 ATOM 1212 CG2 ILE 1006 37.602 14.777 -0.103 1.00 12.82 ATOM 1213 CG1 ILE 1006 35.718 13.341 0.441 1.00 20.16 ATOM 1214 CD1 ILE 1006 35.961 12.446 -0.834 1.00 11.88 ATOM 1215 C ILE 1006 35.998 17.136 1.377 1.00 22.88 ATOM 1216 O ILE 1006 37.113 17.730 1.431 1.00 21.25 ATOM 1217 N CYS 1007 34.854 17.788 1.108 1.00 21.47 ATOM 1219 CA CYS 1007 34.860 19.240 0.909 1.00 21.66 ATOM 1220 CB CYS 1007 33.522 19.825 0.431 1.00 24.87 ATOM 1221 SG CYS 1007 33.760 21.544 -0.085 1.00 30.17 ATOM 1222 C CYS 1007 35.247 19.953 2.196 1.00 22.22 ATOM 1223 O CYS 1007 36.024 20.905 2.158 1.00 25.94 ATOM 1224 N TYR 1008 34.691 19.527 3.331 1.00 20.53 ATOM 1226 CA TYR 1008 35.030 20.132 4.617 1.00 17.94 ATOM 1227 CB TYR 1008 34.248 19.493 5.758 1.00 18.61 ATOM 1228 CG TYR 1008 32.753 19.488 5.626 1.00 17.97 ATOM 1229 CD1 TYR 1008 32.019 18.455 6.175 1.00 16.67 ATOM 1230 CE1 TYR 1008 30.641 18.462 6.158 1.00 22.78 ATOM 1231 CD2 TYR 1008 32.059 20.549 5.031 1.00 22.19 ATOM 1232 CE2 TYR 1008 30.646 20.569 5.011 1.00 20.60 ATOM 1233 CZ TYR 1008 29.949 19.513 5.579 1.00 23.22 ATOM 1234 OH TYR 1008 28.574 19.454 5.551 1.00 18.30 ATOM 1236 C TYR 1008 36.537 19.945 4.883 1.00 18.55 ATOM 1237 O TYR 1008 37.217 20.917 5.256 1.00 20.35 ATOM 1238 N SER 1009 37.056 18.726 4.642 1.00 14.74 ATOM 1240 CA SER 1009 38.476 18.409 4.852 1.00 13.39 ATOM 1241 CB SER 1009 38.810 16.962 4.473 1.00 17.24 ATOM 1242 OG SER 1009 38.018 16.001 5.152 1.00 26.04 ATOM 1244 C SER 1009 39.310 19.309 3.985 1.00 16.36 ATOM 1245 O SER 1009 40.317 19.864 4.446 1.00 20.21 ATOM 1246 N PHE 1010 38.953 19.375 2.699 1.00 20.97 ATOM 1248 CA PHE 1010 39.654 20.246 1.742 1.00 23.34 ATOM 1249 CB PHE 1010 38.985 20.126 0.365 1.00 18.83 ATOM 1250 CG PHE 1010 39.605 21.002 -0.685 1.00 17.13 ATOM 1251 CD1 PHE 1010 38.830 21.940 -1.370 1.00 13.94 ATOM 1252 CD2 PHE 1010 40.979 20.918 -0.968 1.00 17.85 ATOM 1253 CE1 PHE 1010 39.410 22.804 -2.339 1.00 16.30 ATOM 1254 CE2 PHE 1010 41.569 21.763 -1.917 1.00 17.15 ATOM 1255 CZ PHE 1010 40.772 22.714 -2.608 1.00 18.02

## FIG. 7(25)

ATOM 1256 C PHE 1010 39.688 21.746 2.242 1.00 22.02 ATOM 1257 O PHE 1010 40.749 22.390 2.298 1.00 23.00 ATOM 1258 N GLN 1011 38.535 22.271 2.643 1.00 19.25 ATOM 1260 CA GLN 1011 38.418 23.640 3.159 1.00 19.07 ATOM 1261 CB GLN 1011 36.980 23.945 3.480 1.00 12.84 ATOM 1262 CG GLN 1011 36.117 24.005 2.270 1.00 6.53 ATOM 1263 CD GLN 1011 34.713 24.371 2.659 1.00 18.81 ATOM 1264 OE1 GLN 1011 34.490 25.382 3.347 1.00 21.22 ATOM 1265 NE2 GLN 1011 33.760 23.525 2.302 1.00 26.88 ATOM 1268 C GLN 1011 39.262 23.894 4.394 1.00 18.28 ATOM 1269 O GLN 1011 39.840 24.982 4.543 1.00 19.80 ATOM 1270 N VAL 1012 39.270 22.934 5.319 1.00 11.82 ATOM 1272 CA VAL 1012 40.110 23.063 6.500 1.00 13.54 ATOM 1273 CB VAL 1012 39.825 21.936 7.528 1.00 15.67 ATOM 1274 CG1 VAL 1012 40.686 22.107 8.795 1.00 10.56 ATOM 1275 CG2 VAL 1012 38.370 21.948 7.901 1.00 14.92 ATOM 1276 C VAL 1012 41.618 23.068 6.068 1.00 16.72 ATOM 1277 O VAL 1012 42.448 23.782 6.665 1.00 20.48 ATOM 1278 N ALA 1013 42.001 22.291 5.051 1.00 15.90 ATOM 1280 CA ALA 1013 43.401 22.352 4.602 1.00 17.77 ATOM 1281 CB ALA 1013 43.732 21.206 3.638 1.00 10.59 ATOM 1282 C ALA 1013 43.685 23.755 3.963 1.00 15.74 ATOM 1283 O ALA 1013 44.764 24.302 4.139 1.00 17.49 ATOM 1284 N LYS 1014 42.718 24.342 3.244 1.00 17.18 ATOM 1286 CA LYS 1014 42.866 25.706 2.665 1.00 15.11 ATOM 1287 CB LYS 1014 41.557 26.152 2.020 1.00 23.73 ATOM 1288 CG LYS 1014 41.146 25.474 0.748 1.00 23.57 ATOM 1289 CD LYS 1014 41.963 26.033 -0.354 1.00 26.38 ATOM 1290 CE LYS 1014 41.172 25.978 -1.617 1.00 38.71 ATOM 1291 NZ LYS 1014 42.034 26.404 -2.776 1.00 50.36 ATOM 1295 C LYS 1014 43.105 26.678 3.823 1.00 11.16 ATOM 1296 O LYS 1014 44.066 27.452 3.818 1.00 13.85 ATOM 1297 N GLY 1015 42.210 26.590 4.816 1.00 10.82 ATOM 1299 CA GLY 1015 42.250 27.403 6.017 1.00 12.48 ATOM 1300 C GLY 1015 43.584 27.327 6.715 1.00 17.17 ATOM 1301 O GLY 1015 44.124 28.349 7.130 1.00 19.92 ATOM 1302 N MET 1016 45.426 25.927 7.439 1.00 17.82 45.516 24.488 7.925 1.00 17.77 44.538 24.156 9.057 44.159 26.128 6.763 1.00 17.82 ATOM 1304 CA MET 1016 ATOM 1305 CB MET 1016 ATOM 1306 CG MET 1016 ATOM 1307 SD MET 1016 44.931 24.991 10.623 1.00 15.49

## FIG. 7(26)

ATOM 1308 CE MET 1016 46.642 24.894 10.658 1.00 5.63 ATOM 1309 C MET 1016 46.625 26.321 6.618 1.00 14.62 ATOM 1310 O MET 1016 47.680 26.667 7.163 1.00 15.76 ATOM 1311 N GLU 1017 46.487 26.208 5.305 1.00 14.65 ATOM 1313 CA GLU 1017 47.552 26.608 4.384 1.00 21.43 ATOM 1314 CB GLU 1017 47.177 26.195 2.947 1.00 21.43 ATOM 1315 CG GLU 1017 48.162 26.622 1.878 1.00 22.82 ATOM 1316 CD GLU 1017 47.634 26.421 0.436 1.00 27.12 ATOM 1317 OE1 GLU 1017 46.457 26.769 0.141 1.00 24.95 ATOM 1318 OE2 GLU 1017 48.418 25.927 -0.424 1.00 32.93 ATOM 1319 C GLU 1017 47.667 28.145 4.535 1.00 18.38 ATOM 1320 O GLU 1017 48.760 28.668 4.593 1.00 17.43 ATOM 1321 N PHE 1018 46.526 28.839 4.677 1.00 19.09 ATOM 1323 CA PHE 1018 46.509 30.295 4.894 1.00 20.74 ATOM 1324 CB PHE 1018 45.067 30.848 4.870 1.00 27.18 ATOM 1325 CG PHE 1018 44.942 32.338 5.248 1.00 25.91 ATOM 1326 CD1 PHE 1018 44.477 32.718 6.521 1.00 26.19 ATOM 1327 CD2 PHE 1018 45.300 33.345 4.348 1.00 25.16 ATOM 1328 CE1 PHE 1018 44.381 34.059 6.890 1.00 27.10 ATOM 1329 CE2 PHE 1018 45.208 34.708 4.712 1.00 28.34 ATOM 1330 CZ PHE 1018 44.754 35.064 5.982 1.00 26.60 ATOM 1331 C PHE 1018 47.179 30.663 6.216 1.00 18.20 ATOM 1332 O PHE 1018 48.139 31.430 6.228 1.00 15.08 ATOM 1333 N LEU 1019 46.676 30.122 7.328 1.00 16.94 ATOM 1335 CA LEU 1019 47.259 30.414 8.654 1.00 19.44 ATOM 1336 CB LEU 1019 46.673 29.533 9.754 1.00 22.88 ATOM 1337 CG LEU 1019 45.238 29.773 10.165 1.00 24.41 ATOM 1338 CD1 LEU 1019 44.956 28.916 11.388 1.00 24.01 ATOM 1339 CD2 LEU 1019 45.084 31.277 10.485 1.00 25.61 ATOM 1340 C LEU 1019 48.736 30.173 8.660 1.00 19.44 ATOM 1341 O LEU 1019 49.493 30.896 9.316 1.00 18.98 ATOM 1342 N ALA 1020 49.135 29.076 8.023 1.00 19.45 ATOM 1344 CA ALA 1020 50.545 28.747 7.961 1.00 22.29 ATOM 1345 CB ALA 1020 50.748 27.350 7.397 1.00 21.86 ATOM 1346 C ALA 1020 51.252 29.829 7.115 1.00 26.13 ATOM 1347 O ALA 1020 52.348 30.257 7.471 1.00 25.25 ATOM 1348 N SER 1021 50.600 30.323 6.050 1.00 29.72 ATOM 1350 CA SER 1021 51.194 31.384 5.219 1.00 27.59 ATOM 1351 CB SER 1021 50.289 31.754 4.026 1.00 23.95

# FIG. 7(27)

<b>ATOM</b>	1352 OG SER 1021	49.252 32.662	4.349 1.00 22.60
<b>ATOM</b>	1354 C SER 1021	51.469 32.614	6.109 1.00 32.83
<b>ATOM</b>	1355 O SER 1021	52.570 33.172	6.073 1.00 36.57
<b>ATOM</b>	1356 N ARG 1022	50.513 32.957	6.981 1.00 31.88
<b>ATOM</b>	1358 CA ARG 1022	50.645 34.093	7.901 1.00 22.64
<b>ATOM</b>	1359 CB ARG 1022	49.294 34.483	8.465 1.00 17.89
<b>ATOM</b>	1360 CG ARG 1022	48.254 34.691	7.420 1.00 17.72
<b>ATOM</b>	1361 CD ARG 1022	48.648 35.816	6.468 1.00 18.00
<b>ATOM</b>	1362 NE ARG 1022	49.714 36.666	6.993 1.00 31.94
<b>ATOM</b>	1364 CZ ARG 1022	49.625 37.980	7.168 1.00 30.72
<b>ATOM</b>	1365 NH1 ARG 1022	50.653 38.644	7.662 1.00 23.85
<b>ATOM</b>	1368 NH2 ARG 1022	48.508 38.620	6.862 1.00 40.00
<b>ATOM</b>	1371 C ARG 1022	51.563 33.787	9.056 1.00 24.84
<b>ATOM</b>	1372 O ARG 1022	51.718 34.612	9.960 1.00 23.27
<b>ATOM</b>	1373 N LYS 1023	52.115 32.576	9.061 1.00 23.84
<b>ATOM</b>	1375 CA LYS 1023	53.039 32.137	10.094 1.00 23.59
<b>ATOM</b>	1376 CB LYS 1023	54.237 33.067	10.196 1.00 22.44
<b>ATOM</b>	1377 C LYS 1023	52.404 31.899	11.456 1.00 25.21
<b>ATOM</b>	1378 O LYS 1023	53.054 32.024	12.504 1.00 28.54
<b>ATOM</b>	1379 N CYS 1024	51.164 31.435	11.411 1.00 20.82
<b>ATOM</b>	1381 CA CYS 1024	50.404 31.114	12.595 1.00 28.12
<b>ATOM</b>	1382 CB CYS 1024	48.982 31.709	12.472 1.00 30.32
<b>ATOM</b>	1383 SG CYS 1024	48.936 33.504	12.847 1.00 33.73
<b>ATOM</b>	1384 C CYS 1024	50.388 29.576	12.729 1.00 32.20
<b>ATOM</b>	1385 O CYS 1024	50.636 28.882	11.756 1.00 38.70
<b>ATOM</b>	1386 N ILE 1025	50.167 29.057	13.934 1.00 30.55
<b>ATOM</b>	1388 CA ILE 1025	50.123 27.619	14.216 1.00 33.60
<b>ATOM</b>	1389 CB ILE 1025	51.406 27.169	14.970 1.00 36.10
<b>ATOM</b>	1390 CG2 ILE 1025	51.223 25.807	15.619 1.00 38.88
ATOM	1391 CG1 ILE 1025	52.585 27.121	13.988 1.00 38.38
ATOM	1392 CD1 ILE 1025	53.913 27.422	14.604 1.00 34.51
<b>ATOM</b>	1393 C ILE 1025		15.104 1.00 33.66
ATOM	1394 O ILE 1025		16.034 1.00 41.71
	1395 N HIS 1026	47.958 26.643	14.797 1.00 31.27
ATOM	1397 CA HIS 1026		15.589 1.00 27.97
ATOM	1398 CB HIS 1026		14.861 1.00 23.43
ATOM	1399 CG HIS 1026		15.229 1.00 30.06
	1400 CD2 HIS 1026		14.560 1.00 33.43
ATOM	1401 ND1 HIS 1026	43.680 25.659	16.393 1.00 24.53

# FIG. 7(28)

<b>ATOM</b>	1403 CE1 HIS 1026	42.428	26.085	16.424	1.00 26.31
<b>ATOM</b>	1404 NE2 HIS 1026	42.199	26.781	15.321	1.00 29.05
<b>ATOM</b>	1406 C HIS 1026	46.901	26.086	17.036	1.00 30.13
<b>ATOM</b>	1407 O HIS 1026	46.335	26.681	17.955	1.00 37.96
<b>ATOM</b>	1408 N ARG 1027	47.662	25.024	17.244	1.00 26.58
<b>ATOM</b>	1410 CA ARG 1027	47.872	24.429	18.583	1.00 31.87
<b>ATOM</b>	1411 CB ARG 1027	48.235	25.483	19.666	1.00 20.17
<b>ATOM</b>	1412 C ARG 1027	46.762	23.449	19.055	1.00 31.55
<b>ATOM</b>	1413 O ARG 1027	47.047	22.477	19.742	1.00 38.11
<b>ATOM</b>	1414 N ASP 1028	45.528	23.629	18.597	1.00 30.85
<b>ATOM</b>	1416 CA ASP 1028	44.466	22.698	18.955	1.00 26.34
<b>ATOM</b>	1417 CB ASP 1028	43.788	23.098	20.248	1.00 32.60
<b>ATOM</b>	1418 CG ASP 1028	42.847	22.020	20.755	1.00 35.64
<b>ATOM</b>	1419 OD1 ASP 1028	41.692	22.346	21.096	1.00 36.08
<b>ATOM</b>	1420 OD2 ASP 1028	43.267	20.842	20.790	1.00 40.39
<b>ATOM</b>	1421 C ASP 1028	43.435	22.565	17.841	1.00 26.23
<b>ATOM</b>	1422 O ASP 1028	42.276	22.926	17.998	1.00 23.40
<b>ATOM</b>	1423 N LEU 1029	43.884	22.034	16.708	1.00 24.88
<b>ATOM</b>	1425- CA LEU 1029	43.053	21.842	15.533	1.00 23.16
<b>ATOM</b>	1426 CB LEU 1029	43.958	21.772	14.299	1.00 18.78
<b>ATOM</b>	1427 CG LEU 1029	43.221	21.714	12.965	1.00 20.21
<b>ATOM</b>	1428 CD1 LEU 1029	42.349	22.952	12.812	1.00 15.13
<b>ATOM</b>	1429 CD2 LEU 1029	44.249	21.601	11.827	1.00 22.91
<b>ATOM</b>	1430 C LEU 1029	42.237	20.562	15.700	1.00 25.25
<b>ATOM</b>	1431 O LEU 1029	42.765	19.473	15.591	1.00 30.47
<b>ATOM</b>	1432 N ALA 1030	40.949	20.703	15.957	1.00 25.99
<b>ATOM</b>	1434 CA ALA 1030	40.062	19.574	16.182	1.00 25.19
<b>ATOM</b>	1435 CB ALA 1030	39.872	19.387	17.679	1.00 24.55
<b>ATOM</b>	1436 C ALA 1030	38.761	20.007	15.558	1.00 27.35
<b>ATOM</b>	1437 O ALA 1030	38.611	21.202	15.302	1.00 33.46
<b>ATOM</b>	1438 N ALA 1031	37.797	19.094	15.379	1.00 25.19
<b>ATOM</b>	1440 CA ALA 1031	36.508	19.451	14.752	1.00 22.16
<b>ATOM</b>	1441 CB ALA 1031	35.772	18.210	14.270	1.00 21.71
<b>ATOM</b>	1442 C ALA 1031	35.551	20.353	15.536	1.00 20.96
<b>ATOM</b>	1443 O ALA 1031	34.639	20.950	14.944	1.00 21.36
<b>ATOM</b>	1444 N ARG 1032	35.712	20.388	16.859	1.00 22.49
ATOM	1446 CA ARG 1032	34.898	21.246	17.736	1.00 27.01
ATOM	1447 CB ARG 1032	35.157	20.945	19.220	1.00 25.22
<b>ATOM</b>	1448 CG- ARG 1032	36.534	21.451	19.707	1.00 34.44
ATOM	1449 CD ARG 1032	37.150	20.503	20.770	1.00 46.39

## FIG. 7(29)

ATOM 1450 NE ARG 1032 38.554 20.752 21.158 1.00 41.28 ATOM 1452 CZ ARG 1032 39.464 19.799 21.352 1.00 32.28 ATOM 1453 NH1 ARG 1032 40.677 20.129 21.709 1.00 27.74 ATOM 1456 NH2 ARG 1032 39.178 18.524 21.148 1.00 31.24 35.296 22.708 17.482 1.00 25.91 ATOM 1459 C ARG 1032 ATOM 1460 O ARG 1032 34.601 23.605 17.935 1.00 30.23 36.451 22.911 16.840 1.00 20.90 ATOM 1461 N ASN 1033 ATOM 1463 CA ASN 1033 37.008 24.222 16.495 1.00 15.77 38.497 24.290 16.813 1.00 18.29 ATOM 1464 CB ASN 1033 ATOM 1465 CG ASN 1033 38.760 24.160 18.254 1.00 20.60 ATOM 1466 OD1 ASN 1033 37.891 24.445 19.067 1.00 29.84 ATOM 1467 ND2 ASN 1033 39.929 23.677 18.601 1.00 18.08 ATOM 1470 C ASN 1033 36.839 24.535 15.019 1.00 19.29 ATOM 1471 O ASN 1033 37.619 25.303 14.450 1.00 17.18 ATOM 1472 N ILE 1034 35.934 23.822 14.366 1.00 17.56 35.631 24.092 12.972 1.00 17.92 ATOM 1474 CA ILE 1034 ATOM 1475 CB ILE 1034 35.813 22.868 12.091 1.00 15.66 ATOM 1476 CG2 ILE 1034 35.364 23.192 10.647 1.00 12.61 ATOM 1477 CG1 ILE 1034 37.247 22.349 12.221 1.00 10.08 ATOM 1478 CD1 ILE 1034 38.312 23.384 11.994 1.00 18.10 ATOM 1479 C ILE 1034 34.147 24.381 13.075 1.00 21.87 ATOM 1480 O ILE 1034 33.410 23.592 13.669 1.00 26.72 ATOM 1481 N LEU 1035 33.711 25.524 12.575 1.00 21.91 32.311 25.883 12.670 1.00 19.45 ATOM 1483 CA LEU 1035 ATOM 1484 CB LEU 1035 32.190 27.310 13.181 1.00 18.73 ATOM 1485 CG LEU 1035 32.102 27.454 14.691 1.00 21.53 ATOM 1486 CD1 LEU 1035 33.019 26.518 15.456 1.00 8.66 ATOM 1487 CD2 LEU 1035 32.391 28.881 15.016 1.00 19.34 ATOM 1488 C LEU 1035 31.700 25.764 11.316 1.00 20.15 ATOM 1489 O LEU 1035 32.377 25.977 10.310 1.00 21.51 ATOM 1490 N LEU 1036 30.429 25.390 11.275 1.00 24.13 29.745 25.237 10.006 1.00 26.96 ATOM 1492 CA LEU 1036 29.027 23.882 9.909 1.00 20.57 ATOM 1493 CB LEU 1036 ATOM 1494 CG LEU 1036 28.149 23.631 8.681 1.00 17.23 ATOM 1495 CD1 LEU 1036 28.877 23.617 7.360 1.00 7.53 27.566 22.306 8.900 1.00 18.85 ATOM 1496 CD2 LEU 1036 ATOM 1497 C LEU 1036 28.827 26.432 9.755 1.00 31.45 27.953 26.794 10.557 1.00 29.93 ATOM 1498 O- LEU 1036 ATOM 1499 N SER 1037 29.094 27.061 8.628 1.00 34.52 28.410 28.248 8.215 1.00 37.11 ATOM 1501 CA SER 1037

### FIG. 7(30)

ATOM 1502 CB SER 1037 29.448 29.220 7.632 1.00 41.11 ATOM 1503 OG SER 1037 28.879 30.439 7.193 1.00 44.80 ATOM 1505 C SER 1037 27.367 27.890 7.209 1.00 39.39 ATOM 1506 O SER 1037 27.045 26.735 7.024 1.00 42.14 ATOM 1507 N GLU 1038 26.884 28.912 6.531 1.00 44.94 ATOM 1509 CA GLU 1038 25.845 28.806 5.534 1.00 50.37 ATOM 1510 CB GLU 1038 25.685 30.152 4.792 1.00 56.15 ATOM 1511 CG GLU 1038 25.599 31.391 5.676 1.00 55.19 ATOM 1512 CD GLU 1038 24.518 31.270 6.708 1.00 59.42 ATOM 1513 OE1 GLU 1038 23.464 30.637 6.419 1.00 58.62 ATOM 1514 OE2 GLU 1038 24.736 31.806 7.816 1.00 63.52 ATOM 1515 C GLU 1038 25.954 27.672 4.518 1.00 51.35 ATOM 1516 O GLU 1038 25.619 26.521 4.816 1.00 57.04 ATOM 1517 N LYS 1039 26.414 27.997 3.317 1.00 46.28 ATOM 1519 CA LYS 1039 26.467 27.021 2.251 1.00 43.05 ATOM 1520 CB LYS 1039 26.455 27.729 0.898 1.00 41.05 ATOM 1521 C LYS 1039 27.689 26.155 2.401 1.00 44.31 ATOM 1522 O LYS 1039 28.687 26.358 1.697 1.00 50.06 ATOM 1523 N ASN 1040 27.611 25.210 3.339 1.00 37.02 ATOM 1525 CA ASN 1040 28.701 24.283 3.630 1.00 32.65 ATOM 1526 CB ASN 1040 28.647 23.041 2.761 1.00 31.69 ATOM 1527 CG ASN 1040 27.641 22.061 3.267 1.00 31.29 ATOM 1528 OD1 ASN 1040 26.740 21.693 2.553 1.00 38.80 ATOM 1529 ND2 ASN 1040 27.749 21.680 4.530 1.00 36.05 ATOM 1532 C ASN 1040 30.096 24.844 3.656 1.00 28.45 ATOM 1533 O ASN 1040 31.079 24.162 3.300 1.00 26.00 ATOM 1534 N VAL 1041 30.174 26.101 4.073 1.00 23.77 ATOM 1536 CA VAL 1041 31.447 26.739 4.207 1.00 16.56 ATOM 1537 CB VAL 1041 31.382 28.274 3.940 1.00 16.16 ATOM 1538 CG1 VAL 1041 32.709 28.948 4.315 1.00 8.57 ATOM 1539 CG2 VAL 1041 31.124 28.509 2.470 1.00 6.79 ATOM 1540 C VAL 1041 31.726 26.382 5.646 1.00 15.50 ATOM 1541 O VAL 1041 30.825 26.333 6.485 1.00 9.73 ATOM 1542 N VAL 1042 32.967 26.022 5.883 1.00 18.82 ATOM 1544 CA VAL 1042 33.431 25.607 7.185 1.00 19.76 ATOM 1545 CB VAL 1042 33.907 24.110 7.051 1.00 22.19 ATOM 1546 CG1 VAL 1042 35.439 23.993 7.041 1.00 18.66 ATOM 1547 CG2 VAL 1042 33.247 23.242 8.100 1.00 22.95 ATOM 1548 C VAL 1042 34.580 26.607 7.483 1.00 20.50 ATOM 1549 O VAL 1042 35.348 26.960 6.575 1.00 17.75

### FIG. 7(31)

34.675 27.082 8.726 1.00 18.30 ATOM 1550 N LYS 1043 35.679 28.070 9.103 1.00 17.43 ATOM 1552 CA LYS 1043 34.977 29.420 9.277 1.00 17.68 ATOM 1553 CB LYS 1043 34.202 29.845 8.031 1.00 19.19 ATOM 1554 CG LYS 1043 33.560 31.228 8.186 1.00 26.86 ATOM 1555 CD LYS 1043 33.270 31.885 6.820 1.00 18.32 ATOM 1556 CE LYS 1043 34.353 32.806 6.425 1.00 22.63 ATOM 1557 NZ LYS 1043 36.373 27.687 10.399 1.00 18.35 ATOM 1561 C LYS 1043 ATOM 1562 O LYS 1043 35.709 27.235 11.330 1.00 17.37 37.692 27.880 10.461 1.00 17.47 ATOM 1563 N ILE 1044 38.504 27.558 11.645 1.00 21.49 ATOM 1565 CA ILE 1044 40.010 27.390 11.267 1.00 20.48 ATOM 1566 CB ILE 1044 40.896 27.250 12.502 1.00 15.75 ATOM 1567 CG2 ILE 1044 40.221 26.237 10.300 1.00 14.66 ATOM 1568 CG1 ILE 1044 41.584 26.344 9.669 1.00 12.76 ATOM 1569 CD1 ILE 1044 38,432 28.735 12.626 1.00 30.73 ATOM 1570 C ILE 1044 38.370 29.888 12.207 1.00 31.68 ATOM 1571 O ILE 1044 38.454 28.436 13.918 1.00 38.50 ATOM 1572 N CYS 1045 38.437 29.444 14.968 1.00 48.73 ATOM 1574 CA CYS 1045 37.027 29.586 15.558 1.00 50.35 ATOM 1575 CB CYS 1045 36.259 28.069 16.173 1.00 59.69 ATOM 1576 SG CYS 1045 39.473 29.041 16.033 1.00 54.63 ATOM 1577 C CYS 1045 39.981 27.912 15.986 1.00 54.88 ATOM 1578 O CYS 1045 39.811 29.954 16.956 1.00 64.20 ATOM 1579 N ASP 1046 40.816 29.700 18.021 1.00 69.98 ATOM 1581 CA ASP 1046 40.454 28.407 18.788 1.00 72.94 ATOM 1582 CB ASP 1046 41.338 28.165 20.009 1.00 75.40 ATOM 1583 CG ASP 1046 40.930 28.584 21.110 1.00 77.66 ATOM 1584 OD1 ASP 1046 42.428 27.547 19.878 1.00 75.18 ATOM 1585 OD2 ASP 1046 42.219 29.580 17.354 1.00 74.21 ATOM 1586 C ASP 1046 ATOM 1587 O ASP 1046 43.183 29.036 17.940 1.00 74.94 42.307 30.205 16.171 1.00 75.46 ATOM 1588 N PHE 1047 43.462 30.212 15.245 1.00 71.53 ATOM 1590 CA PHE 1047 42.919 30.267 13.790 1.00 72.10 ATOM 1591 CB PHE 1047 41.906 31.381 13.526 1.00 71.34 ATOM 1592 CG PHE 1047 42.139 32.327 12.526 1.00 74.26 ATOM 1593 CD1 PHE 1047 40.747 31.501 14.284 1.00 69.46 ATOM 1594 CD2 PHE 1047 41.242 33.367 12.293 1.00 70.87 ATOM 1595 CE1 PHE 1047 39.847 32.533 14.066 1.00 67.97 ATOM 1596 CE2 PHE 1047 40.096 33.467 13.068 1.00 71.41 ATOM 1597 CZ PHE 1047

### FIG. 7(32)

ATOM 1598 C PHE 1047 44.681 31.163 15.426 1.00 67.78 ATOM 1599 O PHE 1047 44.507 32.345 15.797 1.00 63.26 ATOM 1601 CB ASP 1064 29.579 17.003 25.123 1.00 69.86 ATOM 1602 CG ASP 1064 30.534 16.464 24.050 1.00 69.93 31.028 15.321 24.179 1.00 71.35 ATOM 1603 OD1 ASP 1064 ATOM 1604 OD2 ASP 1064 30.776 17.189 23.063 1.00 71.45 ATOM 1605 C ASP 1064 31.511 17.821 26.539 1.00 64.90 ATOM 1606 O ASP 1064 31.512 19.029 26.788 1.00 64.09 ATOM 1609 N ASP 1064 29.229 17.550 27.534 1.00 67.30 ATOM 1611 CA ASP 1064 30.204 17.019 26.533 1.00 67.58 ATOM 1612 N ALA 1065 32.617 17.135 26.278 1.00 61.87 ATOM 1614 CA ALA 1065 33.932 17.759 26.244 1.00 58.06 ATOM 1615 CB ALA 1065 34.479 17.935 27.650 1.00 56.61 ATOM 1616 C ALA 1065 34.888 16.915 25.397 1.00 57.97 ATOM 1617 O ALA 1065 34.491 15.906 24.788 1.00 56.86 ATOM 1618 N ARG 1066 36.155 17.313 25.400 1.00 54.64 ATOM 1620 CA ARG 1066 37.182 16.664 24.607 1.00 50.99 ATOM 1621 CB ARG 1066 37.538 17.539 23.393 1.00 49.53 ATOM 1622 CG ARG 1066 36.459 17.608 22.335 1.00 52.76 ATOM 1623 CD ARG 1066 36.866 16.805 21.125 1.00 57.63 ATOM 1624 NE ARG 1066 35.847 16.645 20.093 1.00 57.02 ATOM 1626 CZ ARG 1066 35.976 17.033 18.824 1.00 55.63 ATOM 1627 NH1 ARG 1066 34.984 16.797 17.995 1.00 57.63 ATOM 1630 NH2 ARG 1066 37.046 17.691 18.385 1.00 40.52 ATOM 1633 C ARG 1066 38.428 16.513 25.427 1.00 49.01 ATOM 1634 O ARG 1066 38.652 17.274 26.364 1.00 46.29 ATOM 1635 N LEU 1067 39.251 15.546 25.041 1.00 46.48 ATOM 1637 CA LEU 1067 40.510 15.320 25.709 1.00 45.62 ATOM 1638 CB LEU 1067 40.703 13.840 26.073 1.00 45.53 ATOM 1639 CG LEU 1067 41.335 13.519 27.441 1.00 44.07 ATOM 1640 CD1 LEU 1067 42,236 12,322 27,273 1.00 37,52 ATOM 1641 CD2 LEU 1067 42.109 14.710 28.057 1.00 39.60 ATOM 1642 C LEU 1067 41.530 15.778 24.677 1.00 42.00 ATOM 1643 O LEU 1067 41.983 15.010 23.832 1.00 41.05 ATOM 1644 N PRO 1068 41.854 17.072 24.698 1.00 41.22 41,265 18,104 25,584 1,00 34,16 ATOM 1645 CD PRO 1068 ATOM 1646 CA PRO 1068 42.817 17.661 23.761 1.00 38.41 ATOM 1647 CB PRO 1068 42.919 19.104 24.277 1.00 36.08 41.496 19.355 24.828 1.00 29.23 ATOM 1648 CG PRO 1068 ATOM 1649 C PRO 1068 44.197 16.961 23.571 1.00 35.36

### FIG. 7(33)

ATOM 1650 O PRO 1068 44.932 17.258 22.623 1.00 37.80 44.552 16.040 24.455 1.00 33.98 ATOM 1651 N LEU 1069 45.829 15.337 24.333 1.00 35.06 ATOM 1653 CA LEU 1069 46.092 14.517 25.601 1.00 37.80 ATOM 1654 CB LEU 1069 47.228 13.497 25.488 1.00 40.67 ATOM 1655 CG LEU 1069 48.599 14.156 25.752 1.00 36.35 ATOM 1656 CD1 LEU 1069 46.939 12.333 26.445 1.00 40.75 ATOM 1657 CD2 LEU 1069 45.776 14.397 23.121 1.00 34.16 ATOM 1658 C LEU 1069 46.787 14.115 22.461 1.00 32.14 ATOM 1659 O LEU 1069 ATOM 1660 N LYS 1070 44.571 13.916 22.859 1.00 28.95 44.280 13.014 21.765 1.00 28.17 ATOM 1662 CA LYS 1070 42.828 12.569 21.911 1.00 22.17 ATOM 1663 CB LYS 1070 42.553 11.730 23.144 1.00 22.02 ATOM 1664 CG LYS 1070 41.085 11.317 23.107 1.00 24.17 ATOM 1665 CD LYS 1070 ATOM 1666 CE LYS 1070 40.851 9.908 23.646 1.00 29.35 39.444 9.436 23.439 1.00 35.82 ATOM 1667 NZ LYS 1070 ATOM 1671 C LYS 1070 44.518 13.582 20.340 1.00 29.26 ATOM 1672 O LYS 1070 44.368 12.867 19.344 1.00 27.81 ATOM 1673 N TRP 1071 44.862 14.865 20.260 1.00 27.00 45.086 15.550 18.995 1.00 27.37 ATOM 1675 CA TRP 1071 ATOM 1676 CB TRP 1071 44.191 16.827 18.882 1.00 20.67 ATOM 1677 CG TRP 1071 42.724 16.551 18.545 1.00 20.12 ATOM 1678 CD2 TRP 1071 41.685 16.138 19.451 1.00 17.97 ATOM 1679 CE2 TRP 1071 40.524 15.892 18.675 1.00 13.02 41.628 15.944 20.838 1.00 23.76 ATOM 1680 CE3 TRP 1071 ATOM 1681 CD1 TRP 1071 42.153 16.560 17.304 1.00 19.50 ATOM 1682 NE1 TRP 1071 40.834 16.155 17.373 1.00 13.62 39.342 15.465 19.233 1.00 16.22 ATOM 1684 CZ2 TRP 1071 40.439 15.511 21.396 1.00 20.67 ATOM 1685 CZ3 TRP 1071 39.321 15.273 20.594 1.00 19.47 ATOM 1686 CH2 TRP 1071 46.523 15.961 18.889 1.00 26.26 ATOM 1687 C TRP 1071 46.948 16.465 17.842 1.00 28.70 ATOM 1688 O TRP 1071 47.278 15.713 19.959 1.00 24.85 ATOM 1689 N MET 1072 ATOM 1691 CA MET 1072 48.676 16.119 20.034 1.00 22.67 49.066 16.317 21.487 1.00 31.30 ATOM 1692 CB MET 1072 48.328 17.416 22.229 1.00 34.64 ATOM 1693 CG MET 1072 48.977 17.610 23.948 1.00 35.65 ATOM 1694 SD MET 1072 50.667 17.842 23.669 1.00 27.97 ATOM 1695 CE MET 1072 ATOM 1696 C MET 1072 49.697 15.215 19.388 1.00 25.43 49.798 14.029 19.729 1.00 21.51 ATOM 1697 O MET 1072

## FIG. 7(34)

ATOM 1698 N ALA 1073 50.545 15.800 18.547 1.00 25.55 ATOM 1700 CA ALA 1073 51.571 15.024 17.874 1.00 29.80 ATOM 1701 CB ALA 1073 52.369 15.912 16.958 1.00 22.65 ATOM 1702 C ALA 1073 52.448 14.453 18.989 1.00 34.88 ATOM 1703 O ALA 1073 52.431 14.970 20.115 1.00 39.38 ATOM 1704 N PRO 1074 53.183 13.355 18.724 1.00 36.01 ATOM 1705 CD PRO 1074 53.087 12.450 17.570 1.00 31.55 ATOM 1706 CA PRO 1074 54.040 12.771 19.769 1.00 36.24 ATOM 1707 CB PRO 1074 54.544 11.485 19.115 1.00 34.34 ATOM 1708 CG PRO 1074 53.415 11.137 18.193 1.00 31.88 ATOM 1709 C PRO 1074 55.189 13.670 20.288 1.00 37.13 ATOM 1710 O PRO 1074 55.570 13.575 21.447 1.00 34.58 ATOM 1711 N GLU 1075 55.746 14.533 19.440 1.00 37.40 ATOM 1713 CA GLU 1075 56.813 15.422 19.884 1.00 40.62 ATOM 1714 CB GLU 1075 57.598 15.990 18.707 1.00 33.55 ATOM 1715 CG GLU 1075 56.853 16.957 17.844 1.00 39.40 ATOM 1716 CD GLU 1075 55,952 16,300 16,828 1,00 43,14 ATOM 1717 OE1 GLU 1075 55.965 15.055 16.720 1.00 49.09 ATOM 1718 OE2 GLU 1075 55.228 17.040 16.124 1.00 44.63 ATOM 1719 C GLU 1075 56.239 16.546 20.757 1.00 42.73 ATOM 1720 O GLU 1075 56.903 17.061 21.639 1.00 44.76 ATOM 1721 N THR 1076 54.982 16.888 20.524 1.00 46.13 ATOM 1723 CA THR 1076 54.304 17.923 21.283 1.00 46.22 ATOM 1724 CB THR 1076 52.991 18.319 20.605 1.00 43.95 ATOM 1725 OG1 THR 1076 53.245 18.666 19.230 1.00 46.46 ATOM 1727 CG2 THR 1076 52.361 19.481 21.334 1.00 43.93 ATOM 1728 C THR 1076 53.991 17.378 22.662 1.00 47.62 ATOM 1729 O THR 1076 54.175 18.057 23.650 1.00 52.45 ATOM 1730 N ILE 1077 53.442 16.173 22.717 1.00 47.96 ATOM 1732 CA ILE 1077 53.123 15.528 23.980 1.00 46.99 ATOM 1733 CB ILE 1077 52.496 14.151 23.720 1.00 46.43 ATOM 1734 CG2 ILE 1077 52.691 13.232 24.895 1.00 46.16 ATOM 1735 CG1 ILE 1077 51.024 14.306 23.384 1.00 44.29 ATOM 1736 CD1 ILE 1077 50.336 13.010 23.163 1.00 46.43 ATOM 1737 C ILE 1077 54.418 15.345 24.767 1.00 51.37 ATOM 1738 O ILE 1077 54.473 15.577 25.974 1.00 52.53 ATOM 1739 N PHE 1078 55.458 14.931 24.058 1.00 53.41 **ATOM 1741 CA PHE 1078** 56.750 14.696 24.672 1.00 58.94 ATOM 1742 CB PHE 1078 57.506 13.570 23.925 1.00 60.74 ATOM 1743 CG PHE 1078 56.901 12.184 24.124 1.00 57.84

### FIG. 7(35)

ATOM 1744 CD1 PHE 1078 56.068 11.612 23.169 1.00 54.09 ATOM 1745 CD2 PHE 1078 57.127 11.483 25.298 1.00 58.64 ATOM 1746 CE1 PHE 1078 55.478 10.380 23.381 1.00 53.82 ATOM 1747 CE2 PHE 1078 56.539 10.254 25.514 1.00 57.20 ATOM 1748 CZ PHE 1078 55.711 9.703 24.555 1.00 55.07 ATOM 1749 C PHE 1078 57.574 15.981 24.767 1.00 63.98 ATOM 1750 O PHE 1078 57.433 16.738 25.736 1.00 67.06 ATOM 1751 N ASP 1079 58.356 16.274 23.724 1.00 66.97 59.215 17.472 23.678 1.00 68.09 ATOM 1753 CA ASP 1079 60.225 17.402 22.501 1.00 66.89 ATOM 1754 CB ASP 1079 60.174 16.082 21.714 1.00 69.02 ATOM 1755 CG ASP 1079 60.254 16.156 20.474 1.00 71.23 ATOM 1756 OD1 ASP 1079 60.089 14.980 22.308 1.00 69.71 ATOM 1757 OD2 ASP 1079 58.434 18.806 23.599 1.00 67.74 ATOM 1758 C ASP 1079 ATOM 1759 O ASP 1079 59.011 19.848 23.266 1.00 66.85 57.137 18.747 23.926 1.00 68.20 ATOM 1760 N ARG 1080 ATOM 1762 CA ARG 1080 56.173 19.858 23.898 1.00 66.60 55.997 20.496 25.279 1.00 67.64 ATOM 1763 CB ARG 1080 54.529 20.758 25.638 1.00 71.26 ATOM 1764 CG ARG 1080 53.823 19.481 26.096 1.00 73.66 ATOM 1765 CD ARG 1080 52.364 19.610 26.226 1.00 75.75 ATOM 1766 NE ARG 1080 51.642 18.981 27.157 1.00 74.86 ATOM 1768 CZ ARG 1080 50.321 19.134 27.211 1.00 69.96 ATOM 1769 NH1 ARG 1080 ATOM 1772 NH2 ARG 1080 52.247 18.212 28.060 1.00 72.78 ATOM 1775 C ARG 1080 56.305 20.920 22.801 1.00 63.93 ATOM 1776 O ARG 1080 55.861 22.069 22.955 1.00 61.93 56.863 20.510 21.667 1.00 61.30 ATOM 1777 N VAL 1081 57.034 21.413 20.545 1.00 58.53 ATOM 1779 CA VAL 1081 58.202 20.951 19.584 1.00 60.54 ATOM 1780 CB VAL 1081 ATOM 1781 CG1 VAL 1081 59.304 20.266 20.370 1.00 62.35 ATOM 1782 CG2 VAL 1081 57.701 20.043 18.455 1.00 55.04 ATOM 1783 C VAL 1081 55.713 21.481 19.771 1.00 56.90 ATOM 1784 O VAL 1081 55.052 20.452 19.560 1.00 57.43 55.287 22.699 19.435 1.00 51.51 ATOM 1785 N TYR 1082 54.078 22.909 18.641 1.00 41.08 ATOM 1787 CA TYR 1082 53.092 23.847 19.332 1.00 37.59 ATOM 1788 CB TYR 1082 ATOM 1789 CG TYR 1082 52.275 23.238 20.442 1.00 32.41 52.800 23.135 21.721 1.00 38.13 ATOM 1790 CD1 TYR 1082 52.043 22.663 22.781 1.00 38.73 ATOM 1791 CE1 TYR 1082 50.961 22.843 20.234 1.00 27.91 ATOM 1792 CD2 TYR 1082

### FIG. 7(36)

50.189 22.374 21.287 1.00 33.59 ATOM 1793 CE2 TYR 1082 ATOM 1794 CZ TYR 1082 50.739 22.290 22.572 1.00 36.82 50.001 21.874 23.679 1.00 39.60 ATOM 1795 OH TYR 1082 ATOM 1797 C TYR 1082 54.591 23.598 17.410 1.00 34.81 55.240 24.608 17.545 1.00 33.62 ATOM 1798 O TYR 1082 ATOM 1799 N THR 1083 54.394 22.997 16.236 1.00 34.71 54.819 23.573 14.946 1.00 30.90 ATOM 1801 CA THR 1083 ATOM 1802 CB THR 1083 56.106 22.894 14.384 1.00 29.46 55.789 21.598 13.837 1.00 30.18 ATOM 1803 OG1 THR 1083 ATOM 1805 CG2 THR 1083 57.159 22.768 15.486 1.00 21.74 ATOM 1806 C THR 1083 53.678 23.371 13.946 1.00 27.79 ATOM 1807 O THR 1083 52.651 22.777 14.293 1.00 28.80 ATOM 1808 N ILE 1084 53,804 23,869 12,721 1.00 24,37 52.700 23.615 11.797 1.00 27.69 ATOM 1810 CA ILE 1084 52.739 24.381 10.465 1.00 28.65 ATOM 1811 CB ILE 1084 51.450 25.166 10.284 1.00 29.19 ATOM 1812 CG2 ILE 1084 ATOM 1813 CG1 ILE 1084 53.977 25.259 10.361 1.00 37.75 55.235 24.517 9.985 1.00 46.61 ATOM 1814 CD1 ILE 1084 52.689 22.143 11.459 1.00 26.44 ATOM 1815 C ILE 1084 51.627 21.589 11.173 1.00 24.29 ATOM 1816 O ILE 1084 ATOM 1817 N GLN 1085 53.861 21.507 11.518 1.00 25.11 53.920 20.097 11.188 1.00 24.39 ATOM 1819 CA GLN 1085 55.315 19.612 10.823 1.00 27.61 ATOM 1820 CB GLN 1085 ATOM 1821 CG GLN 1085 55.753 20.012 9.411 1.00 33.25 54.653 19.826 8.347 1.00 34.07 ATOM 1822 CD GLN 1085 53.943 20.779 8.004 1.00 41.60 ATOM 1823 OE1 GLN 1085 54.546 18.632 7.797 1.00 28.88 ATOM 1824 NE2 GLN 1085 53.296 19.267 12.258 1.00 23.23 ATOM 1827 C GLN 1085 52.900 18.141 11.981 1.00 25.97 ATOM 1828 O GLN 1085 ATOM 1829 N SER 1086 53.195 19.798 13.480 1.00 20.86 52.488 19.040 14.507 1.00 18.08 ATOM 1831 CA SER 1086 53.044 19.256 15.926 1.00 20.91 ATOM 1832 CB SER 1086 52.870 20.559 16.440 1.00 21.60 ATOM 1833 OG SER 1086 50.962 19.336 14.353 1.00 20.67 ATOM 1835 C SER 1086 50.138 18.531 14.806 1.00 13.79 ATOM 1836 O SER 1086 ATOM 1837 N ASP 1087 50.602 20.415 13.609 1.00 18.68 49.190 20.793 13.324 1.00 11.08 ATOM 1839 CA ASP 1087 49.038 22.249 12.805 1.00 21.08 ATOM 1840 CB ASP 1087 48.845 23.287 13.920 1.00 23.79 ATOM 1841 CG ASP 1087 49.348 24.407 13.745 1.00 31.01 ATOM 1842 OD1 ASP 1087

## FIG. 7(37)

ATOM 1843 OD2 ASP 1087 48.212 23.013 14.967 1.00 28.91 48.632 19.860 12.261 1.00 11.16 ATOM 1844 C ASP 1087 ATOM 1845 O ASP 1087 47.406 19.640 12.177 1.00 12.65 49.520 19.390 11.390 1.00 9.61 ATOM 1846 N VAL 1088 49.181 18.404 10.345 1.00 13.37 ATOM 1848 CA VAL 1088 ATOM 1849 CB VAL 1088 50.351 18.195 9.389 1.00 15.40 50.057 17.067 8.486 1.00 14.68 ATOM 1850 CG1 VAL 1088 50.609 19.477 8.587 1.00 10.67 ATOM 1851 CG2 VAL 1088 48.839 17.061 11.014 1.00 13.67 ATOM 1852 C VAL 1088 ATOM 1853 O VAL 1088 47.897 16.387 10.618 1.00 15.00 49.618 16.668 12.015 1.00 12.30 ATOM 1854 N TRP 1089 49.301 15.460 12.748 1.00 12.96 ATOM 1856 CA TRP 1089 ATOM 1857 CB TRP 1089 50.236 15.279 13.960 1.00 16.98 49.764 14.195 14.887 1.00 18.14 ATOM 1858 CG TRP 1089 ATOM 1859 CD2 TRP 1089 50.325 12.884 15.031 1.00 18.48 ATOM 1860 CE2 TRP 1089 49.476 12.162 15.893 1.00 20.05 ATOM 1861 CE3 TRP 1089 51.460 12.245 14.503 1.00 22.61 48.640 14.215 15.657 1.00 18.89 ATOM 1862 CD1 TRP 1089 48.451 12.995 16.255 1.00 19.54 ATOM 1863 NE1 TRP 1089 ATOM 1865 CZ2 TRP 1089 49.725 10.839 16.249 1.00 20.08 ATOM 1866 CZ3 TRP 1089 51.709 10.927 14.855 1.00 17.00 ATOM 1867 CH2 TRP 1089 50.846 10.243 15.722 1.00 23.71 47.873 15.711 13.207 1.00 14.68 ATOM 1868 C TRP 1089 ATOM 1869 O TRP 1089 46.987 14.958 12.842 1.00 20.33 ATOM 1870 N SER 1090 47.636 16.823 13.923 1.00 18.59 46.287 17.209 14.413 1.00 15.54 ATOM 1872 CA SER 1090 ATOM 1873 CB SER 1090 46.297 18.603 15.043 1.00 12.20 47.066 18.621 16.237 1.00 18.86 ATOM 1874 OG SER 1090 ATOM 1876 C SER 1090 45.256 17.190 13.309 1.00 16.50 ATOM 1877 O SER 1090 44.128 16.691 13.487 1.00 18.14 ATOM 1878 N PHE 1091 45.635 17.745 12.158 1.00 23.35 ATOM 1880 CA PHE 1091 44.746 17.776 10.997 1.00 20.78 45.445 18.399 9.786 1.00 17.07 ATOM 1881 CB PHE 1091 44.533 18.524 8.598 1.00 21.98 ATOM 1882 CG PHE 1091 43.396 19.347 8.666 1.00 17.34 ATOM 1883 CD1 PHE 1091 44.740 17.754 7.460 1.00 19.42 ATOM 1884 CD2 PHE 1091 42.485 19.398 7.641 1.00 15.43 ATOM 1885 CE1 PHE 1091 ATOM 1886 CE2 PHE 1091 43.829 17.792 6.421 1.00 18.06 42.693 18.618 6.509 1.00 19.76 ATOM 1887 CZ PHE 1091 ATOM 1888 C PHE 1091 44.306 16.332 10.667 1.00 17.25

## FIG. 7(38)

<b>ATOM</b>	1889 O PHE 1091	43.147 16.077 10.334 1.00 15.79
<b>ATOM</b>	1890 N GLY 1092	45.258 15.408 10.812 1.00 19.49
<b>ATOM</b>	1892 CA GLY 1092	45.042 13.988 10.577 1.00 18.11
<b>ATOM</b>	1893 C GLY 1092	44.029 13.429 11.544 1.00 19.35
<b>ATOM</b>	1894 O GLY 1092	43.235 12.581 11.137 1.00 24.23
<b>ATOM</b>	1895 N VAL 1093	44.073 13.836 12.819 1.00 18.53
<b>ATOM</b>	1897 CA VAL 1093	43.055 13.392 13.788 1.00 20.09
<b>ATOM</b>	1898 CB VAL 1093	43.389 13.752 15.298 1.00 15.18
<b>ATOM</b>	1899 CG1 VAL 1093	42.421 13.051 16.187 1.00 17.08
<b>ATOM</b>	1900 CG2 VAL 1093	44.778 13.310 15.698 1.00 11.27
<b>ATOM</b>	1901 C VAL 1093	41.661 13.971 13.376 1.00 22.42
<b>ATOM</b>	1902 O VAL 1093	40.649 13.253 13.396 1.00 26.19
<b>ATOM</b>	1903 N LEU 1094	41.618 15.235 12.938 1.00 23.95
<b>ATOM</b>	1905 CA LEU 1094	40.363 15.893 12.484 1.00 19.63
<b>ATOM</b>	1906 CB LEU 1094	40.667 17.338 12.050 1.00 25.24
<b>ATOM</b>	1907 CG LEU 1094	39.587 18.420 11.974 1.00 27.30
<b>ATOM</b>	1908 CD1 LEU 1094	40.136 19.497 11.113 1.00 28.26
<b>ATOM</b>	1909 CD2 LEU 1094	38.265 17.929 11.385 1.00 27.54
<b>ATOM</b>	1910 C LEU 1094	39.775 15.146 11.280 1.00 16.12
<b>ATOM</b>	1911 O LEU 1094	38.555 15.002 11.129 1.00 16.14
<b>ATOM</b>	1912 N LEU 1095	40.631 14.766 10.348 1.00 16.30
<b>ATOM</b>	1914 CA LEU 1095	40.155 14.003 9.195 1.00 17.98
<b>ATOM</b>	1915 CB LEU 1095	41.321 13.538 8.317 1.00 16.52
<b>ATOM</b>	1916 CG LEU 1095	41.981 14.536 7.386 1.00 14.88
<b>ATOM</b>	1917 CD1 LEU 1095	42.807 13.734 6.399 1.00 11.81
<b>ATOM</b>	1918 CD2 LEU 1095	40.931 15.401 6.639 1.00 21.08
<b>ATOM</b>	1919 C LEU 1095	39.437 12.770 9.722 1.00 17.52
<b>ATOM</b>	1920 O LEU 1095	38.324 12.448 9.270 1.00 16.23
<b>ATOM</b>	1921 N TRP 1096	40.077 12.105 10.697 1.00 14.50
<b>ATOM</b>	1923 CA TRP 1096	39.509 10.916 11.304 1.00 14.02
<b>ATOM</b>	1924 CB TRP 1096	40.452 10.330 12.337 1.00 13.21
<b>ATOM</b>	1925 CG TRP 1096	40.010 8.992 12.850 1.00 18.93
<b>ATOM</b>	1926 CD2 TRP 1096	39.016 8.732 13.856 1.00 24.77
<b>ATOM</b>	1927 CE2 TRP 1096	38.952 7.319 14.020 1.00 27.07
<b>ATOM</b>	1928 CE3 TRP 1096	38.178 9.546 14.647 1.00 29.39
<b>ATOM</b>	1929 CD1 TRP 1096	40.483 7.781 12.460 1.00 21.28
<b>ATOM</b>	1930 NE1 TRP 1096	39.854 6.770 13.154 1.00 18.61
<b>ATOM</b>	1932 CZ2 TRP 1096	38.075 6.700 14.954 1.00 28.21
<b>ATOM</b>	1933 CZ3 TRP 1096	37.303 8.927 15.581 1.00 29.42
<b>ATOM</b>	1934 CH2 TRP 1096	37.266 7.511 15.719 1.00 27.60 <sup>-1</sup>

### FIG. 7(39)

ATOM 1935 C TRP 1096 38.159 11.236 11.927 1.00 18.94 37.212 10.439 11.826 1.00 22.31 ATOM 1936 O TRP 1096 38.046 12.385 12.592 1.00 23.97 ATOM 1937 N GLU 1097 36.754 12.750 13.195 1.00 21.61 ATOM 1939 CA GLU 1097 36.823 14.012 14.041 1.00 26.60 ATOM 1940 CB GLU 1097 ATOM 1941 CG GLU 1097 37.880 14.065 15.109 1.00 21.55 37.795 15.380 15.800 1.00 23.56 ATOM 1942 CD GLU 1097 36.726 15.591 16.393 1.00 21.97 ATOM 1943 OE1 GLU 1097 38.741 16.208 15.706 1.00 20.79 ATOM 1944 OE2 GLU 1097 35.744 13.010 12.116 1.00 19.15 ATOM 1945 C GLU 1097 ATOM 1946 O GLU 1097 34.549 12.766 12.304 1.00 28.35 ATOM 1947 N ILE 1098 36.190 13.565 11.001 1.00 17.99 35.244 13.821 9.915 1.00 17.98 ATOM 1949 CA ILE 1098 35.862 14.650 8.732 1.00 13.59 ATOM 1950 CB ILE 1098 34.880 14.725 7.568 1.00 13.47 ATOM 1951 CG2 ILE 1098 36.169 16.074 9.181 1.00 11.46 ATOM 1952 CG1 ILE 1098 36.691 16.960 8.074 1.00 9.72 ATOM 1953 CD1 ILE 1098 34.645 12.529 9.372 1.00 16.07 ATOM 1954 C ILE 1098 33.444 12.445 9.171 1.00 18.22 ATOM 1955 O ILE 1098 ATOM 1956 N PHE 1099 35.460 11.499 9.171 1.00 20.11 34.925 10.257 8.601 1.00 18.95 ATOM 1958 CA PHE 1099 35.909 9.660 7.625 1.00 16.86 ATOM 1959 CB PHE 1099 36.269 10.584 6.517 1.00 12.61 ATOM 1960 CG PHE 1099 37.308 11.468 6.671 1.00 14.37 ATOM 1961 CD1 PHE 1099 35.522 10.624 5.362 1.00 18.03 ATOM 1962 CD2 PHE 1099 37.595 12.369 5.717 1.00 13.66 ATOM 1963 CE1 PHE 1099 35.811 11.553 4.378 1.00 16.05 ATOM 1964 CE2 PHE 1099 36.843 12.418 4.568 1.00 17.86 ATOM 1965 CZ PHE 1099 34.368 9.201 9.551 1.00 23.18 ATOM 1966 C PHE 1099 34.111 8.070 9.149 1.00 22.90 ATOM 1967 O PHE 1099 34.274 9.553 10.825 1.00 26.68 ATOM 1968 N SER 1100 33.652 8.690 11.820 1.00 24.51 ATOM 1970 CA SER 1100 34.504 8.572 13.079 1.00 25.60 ATOM 1971 CB SER 1100 34.826 9.842 13.625 1.00 29.76 ATOM 1972 OG SER 1100 32.398 9.465 12.145 1.00 26.92 ATOM 1974 C SER 1100 31.765 9.211 13.157 1.00 31.32 ATOM 1975 O SER 1100 32.018 10.387 11.251 1.00 28.15 ATOM 1976 N LEU 1101 . ATOM 1978 CA LEU 1101 30.860 11.241 11.453 1.00 24.97 ATOM 1979 CB LEU 1101 29.556 10.557 11.015 1.00 22.00 29.423 10.410 9.495 1.00 25.66 ATOM 1980 CG LEU 1101

### FIG. 7(40)

28.060 9.866 9.127 1.00 22.23 ATOM 1981 CD1 LEU 1101 29.632 11.768 8.829 1.00 32.30 ATOM 1982 CD2 LEU 1101 30.771 11.779 12.888 1.00 26.64 ATOM 1983 C LEU 1101 29.793 11.552 13.580 1.00 31.34 ATOM 1984 O LEU 1101 31.828 12.446 13.336 1.00 24.93 ATOM 1985 N GLY 1102 31.836 13.057 14.650 1.00 28.61 ATOM 1987 CA GLY 1102 32.129 12.293 15.917 1.00 32.38 ATOM 1988 C GLY 1102 31.647 12.693 16.950 1.00 35.69 ATOM 1989 O GLY 1102 33.004 11.291 15.876 1.00 35.95 ATOM 1990 N ALA 1103 33.354 10.500 17.060 1.00 31.27 ATOM 1992 CA ALA 1103 33.515 9.041 16.672 1.00 36.15 ATOM 1993 CB ALA 1103 34.625 10.972 17.747 1.00 34.29 ATOM 1994 C ALA 1103 35.382 11.788 17.190 1.00 36.92 ATOM 1995 O ALA 1103 34.886 10.417 18.934 1.00 33.11 ATOM 1996 N SER 1104 36.087 10.744 19.715 1.00 35.13 ATOM 1998 CA SER 1104 35.906 10.422 21.207 1.00 38.40 ATOM 1999 CB SER 1104 34.719 10.964 21.765 1.00 50.36 ATOM 2000 OG SER 1104 37.216 9.852 19.249 1.00 34.54 ATOM 2002 C SER 1104 ATOM 2003 O SER 1104 37.039 8.640 19.167 1.00 33.44 38,395 10.434 18.963 1.00 32.93 ATOM 2004 N PRO 1105 38.678 11.877 18.972 1.00 31.54 ATOM 2005 CD PRO 1105 39.571 9.693 18.513 1.00 29.88 ATOM 2006 CA PRO 1105 ATOM 2007 CB PRO 1105 40.633 10.781 18.465 1.00 22.24 39.883 11.965 18.079 1.00 28.04 ATOM 2008 CG PRO 1105 39.919 8.659 19.582 1.00 32.54 ATOM 2009 C PRO 1105 39.480 8.795 20.731 1.00 28.79 ATOM 2010 O PRO 1105 40.700 7.648 19.196 1.00 34.52 ATOM 2011 N TYR 1106 41.148 6.564 20.085 1.00 39.62 ATOM 2013 CA TYR 1106 42.374 6.994 20.896 1.00 37.66 ATOM 2014 CB TYR 1106 43.496 7.566 20.059 1.00 39.50 ATOM 2015 CG TYR 1106 43.690 8.957 19.976 1.00 37.50 ATOM 2016 CD1 TYR 1106 44.655 9.518 19.143 1.00 35.61 ATOM 2017 CE1 TYR 1106 44.315 6.739 19.293 1.00 34.54 ATOM 2018 CD2 TYR 1106 45.305 7.290 18.446 1.00 38.80 ATOM 2019 CE2 TYR 1106 45.466 8.686 18.373 1.00 38.23 ATOM 2020 CZ TYR 1106 46.412 9.240 17.520 1.00 31.37 ATOM 2021 OH TYR 1106 40.022 6.128 21.016 1.00 47.24 ATOM 2023 C TYR 1106 40.100 6.296 22.247 1.00 46.94 ATOM 2024 O TYR 1106 38.947 5.570 20.431 1.00 52.30 ATOM 2025 N PRO 1107 38.880 5.234 18.996 1.00 52.76 ATOM 2026 CD PRO 1107

### FIG. 7(41)

37.750 5.088 21.125 1.00 55.67 ATOM 2027 CA PRO 1107 37.078 4.223 20.066 1.00 55.09 ATOM 2028 CB PRO 1107 37.420 4.931 18.797 1.00 52.62 ATOM 2029 CG PRO 1107 38.035 4.300 22.408 1.00 60.55 ATOM 2030 C PRO 1107 38.668 3.231 22.377 1.00 60.88 ATOM 2031 O PRO 1107 37.631 4.894 23.533 1.00 62.85 ATOM 2032 N GLY 1108 37.790 4.284 24.845 1.00 63.10 ATOM 2034 CA GLY 1108 39.171 3.783 25.228 1.00 61.44 ATOM 2035 C GLY 1108 ATOM 2036 O GLY 1108 39.319 3.010 26.178 1.00 63.49 40.181 4.228 24.498 1.00 58.31 ATOM 2037 N VAL 1109 41.548 3.835 24.766 1.00 55.54 ATOM 2039 CA VAL 1109 42.430 4.181 23.580 1.00 54.11 ATOM 2040 CB VAL 1109 43.857 3.787 23.857 1.00 51.33 ATOM 2041 CG1 VAL 1109 41.875 3.528 22.306 1.00 54.09 ATOM 2042 CG2 VAL 1109 42.006 4.657 25.949 1.00 57.04 ATOM 2043 C VAL 1109 41.492 5.749 26.163 1.00 57.18 ATOM 2044 O VAL 1109 42.969 4.140 26.711 1.00 59.43 ATOM 2045 N LYS 1110 43,497 4.849 27.880 1.00 60.27 ATOM 2047 CA LYS 1110 43.928 3.842 28.936 1.00 63.70 ATOM 2048 CB LYS 1110 44.664 5.796 27.538 1.00 60.52 ATOM 2049 C LYS 1110 45.570 5.410 26.780 1.00 61.06 ATOM 2050 O LYS 1110 44.665 7.006 28.115 1.00 58.79 ATOM 2051 N ILE 1111 45.732 7.987 27.859 1.00 60.01 ATOM 2053 CA ILE 1111 45.236 9.441 27.886 1.00 63.41 ATOM 2054 CB ILE 1111 44.517 9.798 26.596 1.00 58.31 ATOM 2055 CG2 ILE 1111 44.413 9.688 29.145 1.00 69.87 ATOM 2056 CG1 ILE 1111 44.341 11.144 29.528 1.00 75.64 ATOM 2057 CD1 ILE 1111 46.949 7.891 28.781 1.00 58.91 ATOM 2058 C ILE 1111 47.670 8.862 28.992 1.00 59.56 ATOM 2059 O ILE 1111 47.187 6.697 29.299 1.00 60.43 ATOM 2060 N ASP 1112 48.312 6.407 30.173 1.00 56.25 ATOM 2062 CA ASP 1112 48.318 4.919 30.421 1.00 59.88 ATOM 2063 CB ASP 1112 48.273 4.131 29.122 1.00 67.87 ATOM 2064 CG ASP 1112 47.179 3.893 28.564 1.00 71.34 ATOM 2065 OD1 ASP 1112 49.348 3.765 28.628 1.00 72.11 ATOM 2066 OD2 ASP 1112 49.612 6.795 29.489 1.00 54.37 ATOM 2067 C ASP 1112 49.634 7.066 28.284 1.00 50.67 -ATOM 2068 O ASP 1112 50.710 6.741 30.236 1.00 55.36 ATOM 2069 N GLU 1113 52.024 7.089 29.683 1.00 55.99 ATOM 2071 CA GLU 1113 53.051 7.374 30.806 1.00 58.69 ATOM 2072 CB GLU 1113

# FIG. 7(42)

ATOM	2073 C GLU 1113	52.552	6.015	28.726	1.00 54.42
<b>ATOM</b>	2074 O GLU 1113	53.624	6.175	28.126	1.00 51.91
<b>ATOM</b>	2075 N GLU 1114	51.822	4.903	28.627	1.00 51.54
<b>ATOM</b>	2077 CA GLU 1114	52.192	3.819	27.719	1.00 54.36
<b>ATOM</b>	2078 CB GLU 1114	51.873	2.452	28.322	1.00 56.43
<b>ATOM</b>	2079 CG GLU 1114	53.072	1.749	28.948	1.00 63.29
<b>ATOM</b>	2080 CD GLU 1114	53.996	2.661	29.772	1.00 67.36
<b>ATOM</b>	2081 OE1 GLU 1114	55.153	2.870	29.329	1.00 67.34
<b>ATOM</b>	2082 OE2 GLU 1114	53.590	3.127	30.873	1.00 68.20
<b>ATOM</b>	2083 C GLU 1114	51.440	4.031	26.412	1.00 52.22
<b>ATOM</b>	2084 O GLU 1114	51.830	3.514	25.360	1.00 51.74
<b>ATOM</b>	2085 N PHE 1115	50.383	4.840	26.486	1.00 49.67
<b>ATOM</b>	2087 CA PHE 1115	49.603	5.175	25.320	1.00 44.59
<b>ATOM</b>	2088 CB PHE 1115	48.400	6.013		1.00 44.73
<b>ATOM</b>	2089 CG PHE 1115	47.918			1.00 49.93
<b>ATOM</b>	2090 CD1 PHE 1115	48.140		24.621	1.00 50.02
<b>ATOM</b>	2091 CD2 PHE 1115	47.251		23.477	1.00 53.38
<b>ATOM</b>	2092 CE1 PHE 1115	47.704			1.00 52.88
<b>ATOM</b>	2093 CE2 PHE 1115	46.805			1.00 51.00
<b>ATOM</b>	2094 CZ PHE 1115	47.033	8.535	22.474	1.00 54.64
<b>ATOM</b>	2095 C PHE 1115	50.582	5.981	24.507	1.00 46.08
<b>ATOM</b>	2096 O PHE 1115	50.929		23.402	1.00 47.48
<b>ATOM</b>	2097 N CYS 1116	51.127		25.101	1.00 43.91
<b>ATOM</b>	2099 CA CYS 1116	52.109			1.00 45.79
ATOM	2100 CB CYS 1116	52.473			1.00 44.47
ATOM	2101 SG CYS 1116	51.129		26.295	1.00 64.10
ATOM	2102 C CYS 1116	53.392			1.00 46.03
<b>ATOM</b>	2103 O CYS 1116	54.232			1.00 46.86
ATOM	2104 N ARG 1117	53.536	5.911		1.00 44.91
ATOM	2106 CA ARG 1117	54.688			1.00 41.89
<b>ATOM</b>	2107 CB ARG 1117	54.882	4.001		1.00 43.78
ATOM	2108 CG ARG 1117	56.237			1.00 45.19
ATOM	2109 CD ARG 1117	56.189			1.00 47.09
<b>ATOM</b>					1.00 49.55
ATOM		54.329			1.00 51.59
ATOM		53.783			1.00 51.49
ATOM					1.00 47.17
ATOM					1.00 38.98
ATOM		55.156			1.00 42.49
ATOM	2121 N ARG 1118	53.206	3.751	22.860	1.00 35.52

## FIG. 7(43)

52.745 3.072 21.649 1.00 36.78 ATOM 2123 CA ARG 1118 51.330 2.559 21.880 1.00 31.14 ATOM 2124 CB ARG 1118 51.216 1.675 23.068 1.00 34.41 ATOM 2125 CG ARG 1118 49.766 1.587 23.535 1.00 45.83 ATOM 2126 CD ARG 1118 48.897 0.750 22.693 1.00 53.41 ATOM 2127 NE ARG 1118 47.564 0.658 22.826 1.00 55.58 ATOM 2129 CZ ARG 1118 46.862 -0.144 22.025 1.00 56.70 ATOM 2130 NH1 ARG 1118 46,921 1.380 23.745 1.00 55.55 ATOM 2133 NH2 ARG 1118 52.742 4.067 20.471 1.00 38.92 ATOM 2136 C ARG 1118 53.331 3.835 19.400 1.00 38.28 ATOM 2137 O ARG 1118 52.063 5.186 20.711 1.00 40.67 ATOM 2138 N LEU 1119 51.912 6.295 19.779 1.00 36.71 ATOM 2140 CA LEU 1119 51.192 7.416 20.540 1.00 32.46 ATOM 2141 CB LEU 1119 50.238 8.508 20.049 1.00 25.91 ATOM 2142 CG LEU 1119 51.047 9.651 19.564 1.00 19.62 ATOM 2143 CD1 LEU 1119 49.250 7.993 19.024 1.00 22.26 ATOM 2144 CD2 LEU 1119 53.301 6.728 19.245 1.00 38.89 ATOM 2145 C LEU 1119 53.469 6.960 18.047 1.00 43.59 ATOM 2146 O LEU 1119 54.315 6.771 20.099 1.00 42.22 ATOM 2147 N LYS 1120 55.649 7.152 19.640 1.00 41.56 ATOM 2149 CA LYS 1120 56.523 7.548 20.813 1.00 42.85 ATOM 2150 CB LYS 1120 57.467 8.670 20.467 1.00 52.51 ATOM 2151 CG LYS 1120 58.407 8.989 21.620 1.00 60.23 ATOM 2152 CD LYS 1120 59.298 10.206 21.321 1.00 69.72 ATOM 2153 CE LYS 1120 58.605 11.557 21.283 1.00 76.23 ATOM 2154 NZ LYS 1120 56.351 6.050 18.825 1.00 43.73 ATOM 2158 C LYS 1120 57.287 6.342 18.073 1.00 47.49 ATOM 2159 O LYS 1120 55.892 4.800 18.966 1.00 43.94 ATOM 2160 N GLU 1121 56.453 3.636 18.262 1.00 41.07 ATOM 2162 CA GLU 1121 56.415 2.395 19.147 1.00 48.40 ATOM 2163 CB GLU 1121 57.553 2.283 20.112 1.00 58.39 ATOM 2164 CG GLU 1121 57.183 1.451 21.309 1.00 64.79 ATOM 2165 CD GLU 1121 56.403 0.483 21.119 1.00 67.43 ATOM 2166 OE1 GLU 1121 57.657 1.778 22.431 1.00 67.24 ATOM 2167 OE2 GLU 1121 55.739 3.284 16.968 1.00 39.16 ATOM 2168 C GLU 1121 56.224 2.423 16.216 1.00 39.90 ATOM 2169 O GLU 1121 54.525 3.805 16.781 1.00 31.72 ATOM 2170 N GLY 1122 53.838 3.550 15.531 1.00 22.36 ATOM 2172 CA GLY 1122 52.427 3.064 15.646 1.00 19.85 ATOM 2173 C GLY 1122 51.791 2.779 14.633 1.00 18.01 ATOM 2174 O GLY 1122

### FIG. 7(44)

ATOM 2175 N THR 1123 51.918 2.946 16.860 1.00 16.84 50.535 2.502 16.989 1.00 22.17 ATOM 2177 CA THR 1123 ATOM 2178 CB THR 1123 50.209 2.144 18.469 1.00 29.75 ATOM 2179 OG1 THR 1123 51.148 1.174 18.971 1.00 31.60 ATOM 2181 CG2 THR 1123 48.794 1.587 18.591 1.00 31.44 49.653 3.673 16.453 1.00 23.74 ATOM 2182 C THR 1123 ATOM 2183 O THR 1123 49.940 4.850 16.721 1.00 18.73 ATOM 2184 N ARG 1124 48.597 3.354 15.701 1.00 22.93 47.735 4.379 15.125 1.00 17.39 ATOM 2186 CA ARG 1124 48.094 4.680 13.670 1.00 17.70 ATOM 2187 CB ARG 1124 ATOM 2188 CG ARG 1124 49.478 5.192 13.406 1.00 14.57 49.713 6.484 14.040 1.00 14.31 ATOM 2189 CD ARG 1124 51.046 6.935 13.684 1.00 10.98 ATOM 2190 NE ARG 1124 52.067 6.988 14.533 1.00 16.02 ATOM 2192 CZ ARG 1124 51.861 6.604 15.775 1.00 10.96 ATOM 2193 NH1 ARG 1124 ATOM 2196 NH2 ARG 1124 53.269 7.468 14.163 1.00 8.74 46.317 3.893 15.096 1.00 16.31 ATOM 2199 C ARG 1124 ATOM 2200 O ARG 1124 46.085 2.698 15.022 1.00 20.38 45.380 4.847 15.081 1.00 21.15 ATOM 2201 N MET 1125 43,943 4.570 15.023 1.00 23.81 ATOM 2203 CA MET 1125 43.158 5.870 15.012 1.00 16.88 ATOM 2204 CB MET 1125 42.783 6.397 16.380 1.00 17.08 ATOM 2205 CG MET 1125 41.656 7.825 16.270 1.00 25.19 ATOM 2206 SD MET 1125 ATOM 2207 CE MET 1125 42.908 9.123 15.776 1.00 17.02 43.604 3.789 13.749 1.00 29.80 ATOM 2208 C MET 1125 44.298 3.923 12.748 1.00 33.37 ATOM 2209 O MET 1125 ATOM 2210 N ARG 1126 42,576 2.953 13.806 1.00 36.07 ATOM 2212 CA ARG 1126 42.116 2.183 12.668 1.00 36.36 41.465 0.859 13.154 1.00 40.10 ATOM 2213 CB ARG 1126 40.257 1.021 14.061 1.00 54.46 ATOM 2214 CG ARG 1126 38.956 1.268 13.263 1.00 65.08 ATOM 2215 CD ARG 1126 37.839 1.758 14.091 1.00 72.39 ATOM 2216 NE ARG 1126 36.545 1.753 13.740 1.00 74.53 ATOM 2218 CZ ARG 1126 35.636 2.233 14.588 1.00 78.72 ATOM 2219 NH1 ARG 1126 ATOM 2222 NH2 ARG 1126 36.140 1.267 12.562 1.00 74.28 ATOM 2225 C ARG 1126 41.124 3.094 11.888 1.00 32.52 40.706 4.117 12.380 1.00 34.88 ATOM 2226 O ARG 1126 ATOM 2227 N ALA 1127 40.760 2.725 10.676 1.00 29.80 39.888 3.508 9.812 1.00 29.83 ATOM 2229 CA ALA 1127 39.743 2.782 8.460 1.00 32.24 ATOM 2230 CB ALA 1127

### FIG. 7(45)

38.518 3.697 10.415 1.00 34.29 ATOM 2231 C ALA 1127 ATOM 2232 O ALA 1127 37.944 2.727 10.881 1.00 39.95 ATOM 2233 N PRO 1128 37.943 4.934 10.335 1.00 34.66 ATOM 2234 CD PRO 1128 38.477 6.142 9.685 1.00 35.04 ATOM 2235 CA PRO 1128 36.612 5.251 10.871 1.00 31.59 36.511 6.776 10.669 1.00 32.56 ATOM 2236 CB PRO 1128 37.819 7.222 10.499 1.00 31.06 ATOM 2237 CG PRO 1128 35.648 4.597 9.916 1.00 33.99 ATOM 2238 C PRO 1128 35.975 4.429 8.749 1.00 38.28 ATOM 2239 O PRO 1128 ATOM 2240 N ASP 1129 34.416 4.371 10.344 1.00 31.98 33.425 3.728 9.489 1.00 34.11 ATOM 2242 CA ASP 1129 32.157 3.432 10.277 1.00 29.91 ATOM 2243 CB ASP 1129 ATOM 2244 CG ASP 1129 32.447 2.811 11.623 1.00 34.04 ATOM 2245 OD1 ASP 1129 33.519 2.172 11.805 1.00 35.22 31.597 2.976 12.515 1.00 36.43 ATOM 2246 OD2 ASP 1129 ATOM 2247 C ASP 1129 33.061 4.360 8.158 1.00 35.75 32.441 3.699 7.312 1.00 38.26 ATOM 2248 O ASP 1129 ATOM 2249 N TYR 1130 33.444 5.613 7.925 1.00 32.58 33.056 6.200 6.649 1.00 34.86 ATOM 2251 CA TYR 1130 ATOM 2252 CB TYR 1130 32.067 7.332 6.888 1.00 38.26 ATOM 2253 CG TYR 1130 30.996 6.960 7.889 1.00 37.51 31.208 7.153 9.245 1.00 36.44 ATOM 2254 CD1 TYR 1130 ATOM 2255 CE1 TYR 1130 30,249 6.853 10.148 1.00 40.00 29.787 6.442 7.468 1.00 39.18 ATOM 2256 CD2 TYR 1130 28.813 6.143 8.360 1.00 34.53 ATOM 2257 CE2 TYR 1130 29.050 6.353 9.709 1.00 39.16 ATOM 2258 CZ TYR 1130 ATOM 2259 OH TYR 1130 28.120 6.147 10.690 1.00 47.34 ATOM 2261 C TYR 1130 34.136 6.657 5.732 1.00 34.80 33.853 7.257 4.694 1.00 27.05 ATOM 2262 O TYR 1130 35.388 6.414 6.108 1.00 37.58 ATOM 2263 N THR 1131 ATOM 2265 CA THR 1131 36.457 6.829 5.238 1.00 38.70 ATOM 2266 CB THR 1131 37.783 6.598 5.763 1.00 39.57 37.775 5.417 6.564 1.00 51.23 ATOM 2267 OG1 THR 1131 38.250 7.775 6.481 1.00 49.58 ATOM 2269 CG2 THR 1131 36.476 6.071 3.955 1.00 38.19 ATOM 2270 C THR 1131 ATOM 2271 O THR 1131 35.913 4.967 3.808 1.00 38.82 37.297 6.649 3.104 1.00 31.58 ATOM 2272 N THR 1132 . 37.638 6.148 1.836 1.00 27.37 ATOM 2274 CA THR 1132 37.591 7.302 0.887 1.00 18.06 ATOM 2275 CB THR 1132 36.274 7.366 0.348 1.00 29.75 ATOM 2276 OG1 THR 1132

## FIG. 7(46)

ATOM 2278 CG2 THR 1132 38.528 7.126 -0.161 1.00 32.09 ATOM 2279 C THR 1132 39.064 5.634 2.159 1.00 31.18 ATOM 2280 O THR 1132 39.678 6.088 - 3.149 1.00 37.35 ATOM 2281 N PRO 1133 39.543 4.601 1.439 1.00 29.49 ATOM 2282 CD PRO 1133 38.884 3.875 0.336 1.00 28.18 40.876 4.065 1.686 1.00 23.60 ATOM 2283 CA PRO 1133 ATOM 2284 CB PRO 1133 41.029 2.998 0.604 1.00 29.05 ATOM 2285 CG PRO 1133 39.640 2.581 0.319 1.00 28.36 ATOM 2286 C PRO 1133 41.917 5.122 1.500 1.00 22.87 42.944 5.119 2.182 1.00 30.07 ATOM 2287 O PRO 1133 ATOM 2288 N GLU 1134 41.700 5.983 0.511 1.00 18.80 ATOM 2290 CA GLU 1134 42.656 7.049 0.264 1.00 22.21 ATOM 2291 CB GLU 1134 42.594 7.573 -1.160 1.00 26.28 ATOM 2292 CG GLU 1134 41.214 7.564 -1.765 1.00 40.23 ATOM 2293 CD GLU 1134 40.901 6.347 -2.617 1.00 42.05 ATOM 2294 OE1 GLU 1134 41.727 6.004 -3.504 1.00 44.65 ATOM 2295 OE2 GLU 1134 39.799 5.779 -2.453 1.00 44.07 42.547 8.164 1.300 1.00 21.07 ATOM 2296 C GLU 1134 ATOM 2297 O GLU 1134 43.528 8.877 1.543 1.00 20.78 41.375 8.304 1.940 1.00 20.24 ATOM 2298 N MET 1135 ATOM 2300 CA MET 1135 41.233 9.304 2.996 1.00 16.52 ATOM 2301 CB MET 1135 39.775 9.658 3.319 1.00 17.57 39.158 10.807 2.420 1.00 15.02 ATOM 2302 CG MET 1135 40.199 12.320 2.187 1.00 20.17 ATOM 2303 SD MET 1135 ATOM 2304 CE MET 1135 40.632 12.648 3.877 1.00 13.20 41.974 8.751 4.191 1.00 20.41 ATOM 2305 C MET 1135 ATOM 2306 O MET 1135 42.772 9.461 4.787 1.00 25.79 ATOM 2307 N TYR 1136 41.836 7.448 4.445 1.00 20.30 42.565 6.817 5.540 1.00 17.65 ATOM 2309 CA TYR 1136 ATOM 2310 CB TYR 1136 42.082 5.394 5.832 1.00 21.89 ATOM 2311 CG TYR 1136 42.786 4.775 7.041 1.00 26.17 ATOM 2312 CD1 TYR 1136 42.702 5.353 8.325 1.00 20.81 ATOM 2313 CE1 TYR 1136 43.364 4.781 9.427 1.00 17.33 ATOM 2314 CD2 TYR 1136 43.554 3.612 6.900 1.00 26.03 ATOM 2315 CE2 TYR 1136 44.225 3.034 7.998 1.00 12.75 44.124 3.615 9.245 1.00 16.64 ATOM 2316 CZ TYR 1136 ATOM 2317 OH TYR 1136 44.791 2.999 10.281 1.00 17.57 ATOM 2319 C TYR 1136 44.077 6.847 5.267 1.00 14.28 44.892 7.066 6.179 1.00 19.62 ATOM 2320 O TYR 1136 ATOM 2321 N GLN 1137 44.479 6.693 4.022 1.00 12.55

### FIG. 7(47)

ATOM 2323 CA GLN 1137 45.903 6.777 3.758 1.00 16.34 46.218 6.412 2.325 1.00 18.36 ATOM 2324 CB GLN 1137 ATOM 2325 CG GLN 1137 47.702 6.654 1.945 1.00 21.79 ATOM 2326 CD GLN 1137 48.613 5.655 2.561 1.00 14.21 ATOM 2327 OE1 GLN 1137 48.416 4.469 2.381 1.00 22.64 49.571 6.111 3.344 1.00 18.97 ATOM 2328 NE2 GLN 1137 ATOM 2331 C GLN 1137 46.415 8.193 4.041 1.00 20.40 ATOM 2332 O GLN 1137 47.598 8.378 4.391 1.00 25.11 ATOM 2333 N THR 1138 45.564 9.194 3.807 1.00 18.65 ATOM 2335 CA THR 1138 45.939 10.568 4.068 1.00 15.52 44.921 11.507 3.538 1.00 19.97 ATOM 2336 CB THR 1138 44.797 11.257 2.144 1.00 18.74 ATOM 2337 OG1 THR 1138 45.381 12.939 3.722 1.00 21.70 ATOM 2339 CG2 THR 1138 46.111 10.721 5.566 1.00 12.73 ATOM 2340 C THR 1138 ATOM 2341 O THR 1138 47.067 11.344 6.010 1.00 18.83 ATOM 2342 N MET 1139 45.233 10.118 6.352 1.00 9.32 45.402 10.151 7.809 1.00 12.25 ATOM 2344 CA MET 1139 ATOM 2345 CB MET 1139 44.295 9.349 8.480 1.00 13.21 ATOM 2346 CG MET 1139 42,967 10.007 8.354 1.00 5.60 41.708 8.982 9.003 1.00 17.66 ATOM 2347 SD MET 1139 40.510 9.337 7.925 1.00 2.00 ATOM 2348 CE MET 1139 46.773 9.567 8.198 1.00 15.96 ATOM 2349 C MET 1139 47.573 10.237 8.855 1.00 17.30 ATOM 2350 O MET 1139 ATOM 2351 N LEU 1140 47.058 8.333 7.770 1.00 15.29 ATOM 2353 CA LEU 1140 48.357 7.735 8.081 1.00 14.20 48.542 6.409 7.326 1.00 6.27 ATOM 2354 CB LEU 1140 47.511 5.373 7.745 1.00 15.42 ATOM 2355 CG LEU 1140 47.656 4.103 6.927 1.00 8.64 ATOM 2356 CD1 LEU 1140 47.648 5.103 9.246 1.00 14.99 ATOM 2357 CD2 LEU 1140 49.518 8.684 7.751 1.00 17.20 ATOM 2358 C LEU 1140 50.552 8.691 8.442 1.00 18.73 ATOM 2359 O LEU 1140 49.396 9.413 6.644 1.00 20.16 ATOM 2360 N ASP 1141 50.442 10.374 6.229 1.00 19.52 ATOM 2362 CA ASP 1141 50.139 10.963 4.851 1.00 20.89 ATOM 2363 CB ASP 1141 ATOM 2364 CG ASP 1141 50.228 9.942 3.772 1.00 25.01 50.537 8.765 4.074 1.00 30.17 ATOM 2365 OD1 ASP 1141 49.994 10.321 2.624 1.00 26.42 ATOM 2366 OD2 ASP 1141 ATOM 2367 C ASP 1141 50.627 11.521 7.207 1.00 15.10 51.762 11.905 7.502 1.00 8.73 ATOM 2368 O ASP 1141 49.504 12.101 7.637 1.00 10.75 ATOM 2369 N CYS 1142

## FIG. 7(48)

ATOM 2371 CA CYS 1142 49.516 13.196 8.590 1.00 13.88 ATOM 2372 CB CYS 1142 48.110 13.776 8.739 1.00 17.83 ATOM 2373 SG CYS 1142 47.414 14.574 7.291 1.00 17.66 ATOM 2374 C CYS 1142 50.042 12.717 9.961 1.00 15.52 ATOM 2375 O CYS 1142 50.545 13.513 10.734 1.00 16.31 ATOM 2376 N TRP 1143 49.883 11.424 10.266 1.00 20.06 ATOM 2378 CA TRP 1143 50.344 10.830 11.528 1.00 17.66 ATOM 2379 CB TRP 1143 49.393 9.727 11.991 1.00 15.44 ATOM 2380 CG TRP 1143 48.041 10.236 12.273 1.00 14.25 ATOM 2381 CD2 TRP 1143 46.814 9.495 12.233 1.00 18.13 ATOM 2382 CE2 TRP 1143 45.774 10.401 12.540 1.00 12.59 ATOM 2383 CE3 TRP 1143 46,490 8,143 11,966 1,00 16,02 ATOM 2384 CD1 TRP 1143 47.710 11.514 12.605 1.00 7.90 ATOM 2385 NE1 TRP 1143 46.355 11.618 12.768 1.00 13.52 ATOM 2387 CZ2 TRP 1143 44.425 10.012 12.592 1.00 8.83 ATOM 2388 CZ3 TRP 1143 45.155 7.755 12.017 1.00 11.61 ATOM 2389 CH2 TRP 1143 44.133 8.691 12.327 1.00 16.83 ATOM 2390 C TRP 1143 51.765 10.281 11.442 1.00 23.22 ATOM 2391 O TRP 1143 52.208 9.507 12.298 1.00 27.31 ATOM 2392 N HIS 1144 52.510 10.722 10.440 1.00 24.48 ATOM 2394 CA HIS 1144 53.876 10.280 10.299 1.00 26.08 ATOM 2395 CB HIS 1144 54.495 10.859 9.023 1.00 19.25 ATOM 2396 CG HIS 1144 55.791 10.214 8.654 1.00 18.57 ATOM 2397 CD2 HIS 1144 56.923 10.003 9.374 1.00 14.60 56.016 9.657 7.415 1.00 19.61 ATOM 2398 ND1 HIS 1144 57.231 9.133 7.387 1.00 19.99 ATOM 2400 CE1 HIS 1144 57.803 9.332 8.562 1.00 15.04 ATOM 2401 NE2 HIS 1144 ATOM 2403 C HIS 1144 54.710 10.671 11.542 1.00 32.65 ATOM 2404 O HIS 1144 54.626 11.795 12.031 1.00 31.70 ATOM 2405 N GLY 1145 55.541 9.734 12.016 1.00 37.26 ATOM 2407 CA GLY 1145 56.393 9.970 13.168 1.00 31.32 ATOM 2408 C GLY 1145 57.251 11.212 13.001 1.00 35.04 ATOM 2409 O GLY 1145 57.372 11.989 13.942 1.00 38.42 ATOM 2410 N GLU 1146 57.915 11.373 11.852 1.00 34.51 58.735 12.577 11.598 1.00 37.16 ATOM 2412 CA GLU 1146 ATOM 2413 CB GLU 1146 59.871 12.303 10.627 1.00 37.16 ATOM 2414 CG GLU 1146 61.093 11.742 11.292 1.00 50.26 ATOM 2415 CD GLU 1146 61.186 10.243 11.110 1.00 54.17 ATOM 2416 OE1 GLU 1146 61.158 9.509 12.125 1.00 55.25 ATOM 2417 OE2 GLU 1146 61.280 9.804 9.938 1.00 59.09

## FIG. 7(49)

ATOM 2418 C GLU 1146 57.910 13.742 11.052 1.00 36.46 ATOM 2419 O GLU 1146 57.378 13.665 9.934 1.00 35.72 ATOM 2420 N PRO 1147 57.861 14.868 11.791 1.00 34.09 ATOM 2421 CD PRO 1147 58.490 15.147 13.099 1.00 33.72 57.082 16.020 11.336 1.00 29.77 ATOM 2422 CA PRO 1147 ATOM 2423 CB PRO 1147 57.446 17.106 12.351 1.00 27.86 ATOM 2424 CG PRO 1147 57.668 16.334 13.619 1.00 26.72 ATOM 2425 C PRO 1147 57.436 16.417 9.922 1.00 27.04 ATOM 2426 O PRO 1147 56.559 16.784 9.158 1.00 30.21 ATOM 2427 N SER 1148 58.698 16.255 9.551 1.00 22.56 59.177 16.616 8.210 1.00 24.23 ATOM 2429 CA SER 1148 ATOM 2430 CB SER 1148 60.707 16.724 8.203 1.00 27.40 ATOM 2431 OG SER 1148 61.314 15.477 8.545 1.00 36.19 58.743 15.674 7.101 1.00 21.41 ATOM 2433 C SER 1148 ATOM 2434 O SER 1148 58.890 15.964 5.913 1.00 24.41 58.272 14.508 7.485 1.00 25.45 ATOM 2435 N GLN 1149 ATOM 2437 CA GLN 1149 57.831 13.547 6.497 1.00 26.28 ATOM 2438 CB GLN 1149 58.224 12.142 6.946 1.00 32.79 ATOM 2439 CG GLN 1149 59.705 11.907 6.958 1.00 25.96 ATOM 2440 CD GLN 1149 60.279 12.196 5.622 1.00 32.77 ATOM 2441 OE1 GLN 1149 59.765 11.744 4.591 1.00 36.63 61.312 13.007 5.604 1.00 37.86 ATOM 2442 NE2 GLN 1149 56.327 13.670 6.278 1.00 23.40 ATOM 2445 C GLN 1149 55.783 13.145 5.306 1.00 23.12 ATOM 2446 O GLN 1149 55.662 14.339 7.215 1.00 22.72 ATOM 2447 N ARG 1150 ATOM 2449 CA ARG 1150 54.226 14.581 7.132 1.00 17.86 53.721 15.243 8.392 1.00 16.38 ATOM 2450 CB ARG 1150 ATOM 2451 CG ARG 1150 54.161 14.532 9.598 1.00 13.96 53.285 14.903 10.728 1.00 15.08 ATOM 2452 CD ARG 1150 53.632 14.090 11.879 1.00 24.55 ATOM 2453 NE ARG 1150 54.066 14.564 13.040 1.00 27.63 ATOM 2455 CZ ARG 1150 54.192 15.871 13.230 1.00 27.18 ATOM 2456 NH1 ARG 1150 54.423 13.717 13.991 1.00 29.34 ATOM 2459 NH2 ARG 1150 54.025 15.559 6.008 1.00 16.82 ATOM 2462 C ARG 1150 ATOM 2463 O ARG 1150 54.913 16.382 5.715 1.00 13.09 ATOM 2464 N PRO 1151 52.873 15.464 5.320 1.00 18.01 51.793 14.453 5.320 1.00 6.32 ATOM 2465 CD PRO 1151 52.726 16.442 4.240 1.00 18.95 ATOM 2466 CA PRO 1151 ATOM 2467 CB PRO 1151 51.489 15.948 3.492 1.00 16.01 50.726 15.092 4.520 1.00 10.59 ATOM 2468 CG PRO 1151

## FIG. 7(50)

ATOM 2469 C PRO 1151 52.574 17.861 4.805 1.00 18.27 ATOM 2470 O PRO 1151 52.422 18.039 6.006 1.00 19.70 52.763 18.860 3.958 1.00 19.16 ATOM 2471 N THR 1152 ATOM 2473 CA THR 1152 52.604 20.251 4.366 1.00 14.92 ATOM 2474 CB THR 1152 53.511 21.138 3.560 1.00 13.80 53.146 21.080 2.163 1.00 17.02 ATOM 2475 OG1 THR 1152 ATOM 2477 CG2 THR 1152 54.918 20.697 3.764 1.00 5.40 ATOM 2478 C THR 1152 51.196 20.571 3.979 1.00 13.16 ATOM 2479 O THR 1152 50.682 19.905 3.084 1.00 19.18 ATOM 2480 N PHE 1153 50.561 21.572 4.599 1.00 14.62 ATOM 2482 CA PHE 1153 49.176 21.910 4.224 1.00 12.87 ATOM 2483 CB PHE 1153 48.588 23.023 5.083 1.00 11.95 ATOM 2484 CG PHE 1153 48.157 22.558 6.422 1.00 9.67 ATOM 2485 CD1 PHE 1153 47.037 21.740 6.560 1.00 14.91 ATOM 2486 CD2 PHE 1153 48.891 22.857 7.533 1.00 15.01 ATOM 2487 CE1 PHE 1153 46.660 21.215 7.802 1.00 9.44 ATOM 2488 CE2 PHE 1153 48.529 22.340 8.789 1.00 13.43 ATOM 2489 CZ PHE 1153 47.405 21.513 8.913 1.00 8.41 ATOM 2490 C PHE 1153 49.073 22.253 2.750 1.00 16.98 ATOM 2491 O PHE 1153 48.078 21.927 2.114 1.00 21.60 50.116 22.841 2.168 1.00 15.39 ATOM 2492 N SER 1154 ATOM 2494 CA SER 1154 50.031 23.123 0.754 1.00 17.55 ATOM 2495 CB SER 1154 51.251 23.868 0.254 1.00 25.28 51.244 25.190 0.776 1.00 33.35 ATOM 2496 OG SER 1154 ATOM 2498 C SER 1154 49.850 21.815 0.022 1.00 20.26 ATOM 2499 O SER 1154 48.932 21.704 -0.798 1.00 23.74 50.670 20.808 0.347 1.00 19.47 ATOM 2500 N GLU 1155 ATOM 2502 CA GLU 1155 50.534 19.493 -0.307 1.00 16.55 ATOM 2503 CB GLU 1155 51.588 18.513 0.188 1.00 19.82 ATOM 2504 CG GLU 1155 52.932 18.773 -0.486 1.00 20.20 ATOM 2505 CD GLU 1155 54.128 18.210 0.249 1.00 23.11 ATOM 2506 OE1 GLU 1155 55.226 18.377 -0.312 1.00 35.76 ATOM 2507 OE2 GLU 1155 54.009 17.631 1.359 1.00 21.09 49.153 18.918 -0.107 1.00 16.59 ATOM 2508 C GLU 1155 ATOM 2509 O GLU 1155 48.548 18.414 -1.055 1.00 21.37 ATOM 2510 N LEU 1156 48.619 19.034 1.101 1.00 16.01 ATOM 2512 CA LEU 1156 47.272 18.532 1.375 1.00 18.06 46.969 18.521 2.875 1.00 15.74 ATOM 2513 CB LEU 1156 ATOM 2514 CG LEU 1156 47.688 17.493 3.759 1.00 11.35 47.786 18.049 5.201 1.00 2.08 ATOM 2515 CD1 LEU 1156

### FIG. 7(51)

ATOM 2516 CD2 LEU 1156 46.927 16.150 3.708 1.00 14.36 ATOM 2517 C LEU 1156 46.165 19.287 0.638 1.00 20.03 45.105 18.711 0.355 1.00 26.86 ATOM 2518 O LEU 1156 ATOM 2519 N VAL 1157 46.354 20.570 0.355 1.00 21.44 45.303 21.283 -0.362 1.00 21.15 ATOM 2521 CA VAL 1157 ATOM 2522 CB VAL 1157 45.513 22.801 -0.381 1.00 21.33 ATOM 2523 CG1 VAL 1157 44.569 23.453 -1.368 1.00 15.98 ATOM 2524 CG2 VAL 1157 45.198 23.340 0.974 1.00 13.87 ATOM 2525 C VAL 1157 45.270 20.721 -1.760 1.00 22.88 ATOM 2526 O VAL 1157 44.198 20.508 -2.333 1.00 25.54 ATOM 2527 N GLU 1158 46.445 20.400 -2.282 1.00 23.10 ATOM 2529 CA GLU 1158 46.503 19.815 -3.603 1.00 27.24 ATOM 2530 CB GLU 1158 47.922 19.756 -4.115 1.00 32.82 47.969 18.978 -5.404 1.00 44.73 ATOM 2531 CG GLU 1158 ATOM 2532 CD GLU 1158 49.187 19.268 -6.212 1.00 51.53 49.007 19.887 -7.292 1.00 54.31 ATOM 2533 OE1 GLU 1158 50.298 18.869 -5.765 1.00 51.10 ATOM 2534 OE2 GLU 1158 ATOM 2535 C GLU 1158 45.939 18.403 -3.643 1.00 26.42 45.167 18.051 -4.546 1.00 25.91 ATOM 2536 O GLU 1158 ATOM 2537 N HIS 1159 46.347 17.591 -2.669 1.00 26.36 ATOM 2539 CA HIS 1159 45.897 16.226 -2.611 1.00 21.52 ATOM 2540 CB HIS 1159 46.674 15.444 -1.576 1.00 25.28 ATOM 2541 CG HIS 1159 46.322 13.991 -1.545 1.00 24.66 46.408 13.030 -2.497 1.00 24.44 ATOM 2542 CD2 HIS 1159 45.749 13.387 -0.452 1.00 21.30 ATOM 2543 ND1 HIS 1159 45.489 12.125 -0.731 1.00 23.16 ATOM 2545 CE1 HIS 1159 ATOM 2546 NE2 HIS 1159 45.879 11.884 -1.961 1.00 19.88 44.402 16.104 -2.391 1.00 21.56 ATOM 2548 C HIS 1159 ATOM 2549 O HIS 1159 43,741 15.311 -3.066 1.00 22.19 43.852 16.874 -1.456 1.00 20.25 ATOM 2550 N LEU 1160 ATOM 2552 CA LEU 1160 42.408 16.832 -1.209 1.00 17.66 ATOM 2553 CB LEU 1160 42.111 17.502 0.130 1.00 17.84 42,676 16,760 1.352 1.00 20.17 ATOM 2554 CG LEU 1160 42.472 17.542 2.619 1.00 21.45 ATOM 2555 CD1 LEU 1160 41.992 15.454 1.512 1.00 19.45 ATOM 2556 CD2 LEU 1160 ATOM 2557 C LEU 1160 41.566 17.418 -2.395 1.00 17.71 40.426 17.030 -2.624 1.00 15.39 ATOM 2558 O LEU 1160 ATOM 2559 N GLY 1161 42.130 18.356 -3.153 1.00 23.52 41.434 18.879 -4.322 1.00 21.37 ATOM 2561 CA GLY 1161 41.342 17.741 -5.346 1.00 23.91 ATOM 2562 C GLY 1161

## FIG. 7(52)

ATOM 2563 O GLY 1161 40.295 17.526 -5.971 1.00 23.05 ATOM 2564 N ASN 1162 42.439 16.997 -5.520 1.00 21.49 42.428 15.854 -6.428 1.00 22.31 ATOM 2566 CA ASN 1162 43.771 15.109 -6.427 1.00 22.34 ATOM 2567 CB ASN 1162 44.904 15.888 -7.062 1.00 20.03 ATOM 2568 CG ASN 1162 ATOM 2569 OD1 ASN 1162 44.705 16.903 -7.701 1.00 28.17 46.117 15.401 -6.873 1.00 32.22 ATOM 2570 ND2 ASN 1162 ATOM 2573 C ASN 1162 41.356 14.851 -5.969 1.00 23.05 ATOM 2574 O ASN 1162 40.570 14.378 -6.769 1.00 26.11 ATOM 2575 N LEU 1163 41.360 14.490 -4.688 1.00 21.05 ATOM 2577 CA LEU 1163 40.405 13.523 -4.166 1.00 19.91 ATOM 2578 CB LEU 1163 40.695 13.172 -2.689 1.00 19.18 41.675 12.042 -2.275 1.00 18.62 ATOM 2579 CG LEU 1163 42,959 12,120 -3,020 1,00 24,35 ATOM 2580 CD1 LEU 1163 ATOM 2581 CD2 LEU 1163 41.983 12.043 -0.804 1.00 14.82 39.015 14.038 -4.331 1.00 19.71 ATOM 2582 C LEU 1163 38.110 13.318 -4.767 1.00 23.11 ATOM 2583 O LEU 1163 38.860 15.328 -4.121 1.00 25.91 ATOM 2584 N LEU 1164 ATOM 2586 CA LEU 1164 37.533 15.941 -4.226 1.00 29.28 37.603 17.388 -3.726 1.00 31.25 ATOM 2587 CB LEU 1164 36.348 18.176 -3.371 1.00 25.75 ATOM 2588 CG LEU 1164 ATOM 2589 CD1 LEU 1164 35.429 17.396 -2.435 1.00 31.52 ATOM 2590 CD2 LEU 1164 7.018 15.866 -5.653 1.00 30.07 35.953 15.330 -5.903 1.00 32.61 ATOM 2592 O LEU 1164 ATOM 2593 N GLN 1165 37.810 16.344 -6.598 1.00 33.76 ATOM 2595 CA GLN 1165 37.423 16.317 -8.003 1.00 39.95 38.451 17.048 -8.855 1.00 46.90 ATOM 2596 CB GLN 1165 ATOM 2597 CG GLN 1165 38.758 18.474 -8.480 1.00 49.81 ATOM 2598 CD GLN 1165 39.874 19.024 -9.348 1.00 56.23 ATOM 2599 OE1 GLN 1165 41.056 18.945 -8.997 1.00 55.97 ATOM 2600 NE2 GLN 1165 39.508 19.536 -10.518 1.00 60.66 37.304 14.898 -8.554 1.00 39.33 ATOM 2603 C GLN 1165 36.652 14.685 -9.568 1.00 42.09 ATOM 2604 O GLN 1165 38.059 13.965 -7.988 1.00 36.82 ATOM 2605 N ALA 1166 ATOM 2607 CA ALA 1166 37.994 12.586 -8.441 1.00 34.66 ATOM 2608 CB ALA 1166 39.096 11.748 -7.814 1.00 32.78 ATOM 2609 C ALA 1166 36.640 12.103 -7.991 1.00 36.63 ATOM 2610 O ALA 1166 35.969 11.381 -8.713 1.00 39.47 ATOM 2611 N ASN 1167 36.226 12.532 -6.800 1.00 40.01 34.911 12.158 -6.264 1.00 42.40 ATOM 2613 CA ASN 1167

# FIG. 7(53)

ATOM	2614 CB ASN 1167	34.641 12.878 -4.919 1.00 42.99
<b>ATOM</b>	2615 CG ASN 1167	33.354 12.409 -4.242 1.00 40.80
<b>ATOM</b>	2616 OD1 ASN 1167	32.306 13.046 -4.348 1.00 40.18
<b>ATOM</b>	2617 ND2 ASN 1167	33.436 11.294 -3.532 1.00 36.58
<b>ATOM</b>	2620 C ASN 1167	33.822 12.498 -7.299 1.00 41.88
<b>ATOM</b>	2621 O ASN 1167	32.837 11.789 -7.391 1.00 41.83
<b>ATOM</b>	2622 N ALA 1168	34.057 13.558 -8.085 1.00 45.09
<b>ATOM</b>	2624 CA ALA 1168	33.187 14.065 -9.160 1.00 46.02
<b>ATOM</b>	2625 CB ALA 1168	32.507 12.933 -9.929 1.00 45.92
<b>ATOM</b>	2626 C ALA 1168	32.181 15.123 -8.728 1.00 48.61
<b>ATOM</b>	2628 O ALA 1168	32.627 16.233 -8.363 1.00 50.20
<b>ATOM</b>	2629 O HOH 1	46.858 21.496 16.690 1.00 23.54
<b>ATOM</b>	2632 O HOH 2	49.904 21.605 17.271 1.00 36.65
<b>ATOM</b>	2635 O HOH 3	49.682 18.133 17.657 1.00 50.47
<b>ATOM</b>	2638 O HOH 4	56.606 19.394 15.202 1.00 25.28
<b>ATOM</b>	2641 O HOH 5	57.215 21.949 11.395 1.00 37.66
<b>ATOM</b>	2644 O HOH 6	56.082 25.850 12.933 1.00 34.63
<b>ATOM</b>	2647 O HOH 7	52.355 23.016 6.377 1.00 21.45
<b>ATOM</b>	2650 O HOH 8	51.153 27.376 4.088 1.00 29.93
<b>ATOM</b>	2653 O HOH 9	44.820 28.454 1.120 1.00 16.47
<b>ATOM</b>	2656 O HOH 10	46.377 38.321 5.198 1.00 31.93
<b>ATOM</b>	2659 O HOH 11	43.987 38.133 3.129 1.00 52.41
<b>ATOM</b>	2662 O HOH 12	53.321 40.451 6.702 1.00 31.88
<b>ATOM</b>	2665 O HOH 13	44.977 49.530 8.305 1.00 44.56
<b>ATOM</b>	2668 O HOH 14	44.379 43.338 7.798 1.00 31.72
<b>ATOM</b>	2671 O HOH 15	39.477 40.232 8.468 1.00 36.65
<b>ATOM</b>	2674 O HOH 16	41.987 36.751 10.646 1.00 23.26
<b>ATOM</b>	2677 O HOH 17	41.711 41.873 6.802 1.00 34.79
<b>ATOM</b>	2680 O HOH 18	29.514 24.656 18.739 1.00 31.43
<b>ATOM</b>	2683 O HOH 19	27.493 22.351 15.517 1.00 42.03
<b>ATOM</b>	2686 O HOH 20	24.345 20.097 15.325 1.00 24.92
<b>ATOM</b>	2689 O HOH 21	32.381 18.452 20.520 1.00 75.12
<b>ATOM</b>	2692 O HOH 22	31.071 8.282 19.507 1.00 31.68
<b>ATOM</b>	2695 O HOH 23	33.001 7.742 21.598 1.00 38.67
<b>ATOM</b>	2698 O HOH 24	34.802 6.439 18.667 1.00 34.24
<b>ATOM</b>		32.273 6.932 14.174 1.00 41.21
<b>ATOM</b>	2704 O HOH 26	34.059 5.245 12.870 1.00 49.30
<b>ATOM</b>	2707 O HOH 27	38.059 3.432 4.799 1.00 63.69
<b>ATOM</b>	2710 O HOH 28	41.089 1.841 4.421 1.00 42.86
<b>ATOM</b>	2713 O HOH 29	45.081 9.234 -0.557 1.00 39.97

# FIG. 7(54)

<b>ATOM</b>	2716 O	нон	30	47.301 11.215 1.271 1.00 58.47
<b>ATOM</b>	2719 O	HOH	31	50.046 14.055 0.168 1.00 37.58
<b>ATOM</b>	2722 O	HOH	32	54.425 8.937 4.821 1.00 36.74
<b>ATOM</b>	2725 O	HOH	33	52.279 7.099 5.152 1.00 13.04
<b>ATOM</b>	2728 O	HOH	34	53.025 7.510 7.740 1.00 25.53
<b>ATOM</b>	2731 O	HOH	35	50.852 6.818 10.462 1.00 18.29
<b>ATOM</b>	2734 O	HOH	36	46.448 7.762 15.254 1.00 9.08
<b>ATOM</b>	2737 O	HOH	37	47.326 3.930 20.460 1.00 34.16
<b>ATOM</b>	2740 O	HOH	38	48.264 12.367 20.804 1.00 22.14
<b>ATOM</b>	2743 O	HOH	<b>39</b>	44.276 8.193 24.312 1.00 40.52
<b>ATOM</b>	2746 O	HOH	40	37.491 11.237 25.975 1.00 38.71
<b>ATOM</b>	2749 O	HOH	41	37.592 13.565 23.164 1.00 44.55
<b>ATOM</b>	2752 O	HOH	42	34.887 12.418 26.235 1.00 50.96
<b>ATOM</b>	2755 O	HOH	43	24.823 15.933 17.377 1.00 33.72
<b>ATOM</b>	2758 O	HOH	44	23.302 7.532 7.049 1.00 57.56
<b>ATOM</b>	2761 O	HOH	45	29.954 11.864 -3.109 1.00 38.05
<b>ATOM</b>	2764 O	HOH	46	42.099 3.812 18.044 1.00 40.12
<b>ATOM</b>	2767 O	HOH	47	38.653 0.737 18.003 1.00 37.30
<b>ATOM</b>	2770 O	HOH	48	34.169 14.465 16.707 1.00 20.01
<b>ATOM</b>	2773 O	HOH	49	37.055 32.622 16.570 1.00 31.20
<b>ATOM</b>	2776 O	HOH	50	29.361 31.729 15.460 1.00 21.90
<b>ATOM</b>	2779 O	HOH	51	25.866 31.495 10.192 1.00 24.50
<b>ATOM</b>	2782 O	HOH	52	23.411 32.276 10.616 1.00 68.85
<b>ATOM</b>	2785 O	HOH	53	22.135 37.404 8.648 1.00 40.22
<b>ATOM</b>	2788 O	НОН	54	28.356 36.997 10.747 1.00 22.41
<b>ATOM</b>	2791 O	HOH	55	29.650 33.190 8.897 1.00 31.98
<b>ATOM</b>	2794 O	HOH	56	34.801 35.904 3.297 1.00 59.73
<b>ATOM</b>	2797 O	НОН	57	24.341 20.715 4.934 1.00 28.10
<b>ATOM</b>	2800 O	НОН	58	37.439 20.236 25.832 1.00 33.07
<b>ATOM</b>	2803 O	HOH	59	32.675 51.977 19.122 1.00 33.52
<b>ATOM</b>	2806 O	НОН	60	32.722 54.003 14.118 1.00 25.01
<b>ATOM</b>	2809 O	НОН	61	29.691 54.769 22.004 1.00 27.32
<b>ATOM</b>	2812 O	НОН	62	21.347 47.577 14.711 1.00 27.85
<b>ATOM</b>	2815 O	HOH	63	25.640 44.257 7.516 1.00 24.71
<b>ATOM</b>	2818 O	НОН	64	24.686 40.916 3.785 1.00 55.13
<b>ATOM</b>	2821 O	НОН	65	33.825 48.721 10.105 1.00 39.11
<b>ATOM</b>	2824 O	НОН	66	39.855 54.415 18.247 1.00 50.97
ATOM	2827 O	НОН	-67	36.001 50.053 7.081 1.00 68.99
ATOM	2830 C	НОН	68	37.973 50.651 5.331 1.00 32.12
<b>ATOM</b>	2833 O	НОН	69	40.220 53.227 6.506 1.00 15.02

# FIG. 7(55)

<b>ATOM</b>	2836 O	нон	70	42.258 51.833 6.993 1.00 21.05
ATOM	2839 O	нон	71	36.813 55.217 13.035 1.00 46.29
<b>ATOM</b>	2842 O	нон	<b>72</b>	37.030 55.879 15.712 1.00 39.36
<b>ATOM</b>	2845 O	НОН	73	23.054 45.061 23.607 1.00 51.11
<b>ATOM</b>	2848 O	НОН	74	27.075 54.516 6.971 1.00 51.66
<b>ATOM</b>	2851 O	НОН	<b>75</b>	21.634 54.039 13.651 1.00 36.36
<b>ATOM</b>	2854 O	HOH	76	45.158 47.529 30.699 1.00 56.11
<b>ATOM</b>	2857 O	HOH	77	44.469 45.246 36.699 1.00 36.50
<b>ATOM</b>	2860 O	HOH	<b>78</b>	45.882 41.717 36.085 1.00 28.57
<b>ATOM</b>	2863 O	НОН	<b>79</b>	49.406 41.527 34.292 1.00 65.94
<b>ATOM</b>	2866 O	НОН	80	36.134 49.719 26.101 1.00 63.80
<b>ATOM</b>	2869 O	нон	81	26.884 28.564 16.554 1.00 49.20
<b>ATOM</b>	2872 O	HOH	82	22.079 10.131 13.444 1.00 56.45
<b>ATOM</b>	2875 O	нон	83	41.225 4.655 30.464 1.00 58.98
<b>ATOM</b>	2878 O	HOH	84	47.309 1.568 10.326 1.00 21.69
<b>ATOM</b>	2881 O	HOH	85	56.613 18.335 6.527 1.00 33.97
<b>ATOM</b>	2884 O	нон	86	56.196 16.855 3.275 1.00 47.24
<b>ATOM</b>	2887 O	нон	87	54.826 22.813 0.598 1.00 33.50
<b>ATOM</b>	2890 O	нон	88	52.962 21.915 -2.351 1.00 66.62
ATOM	2893 O	НОН	89	47.896 24.242 -3.714 1.00 40.99
<b>ATOM</b>	2896 O	нон	90	40.295 22.360 25.551 1.00 39.81
<b>ATOM</b>	2899 O	HOH	91	40.188 3.202 15.661 1.00 45.97
<b>ATOM</b>	2902 O	нон	92	45.159 2.965 19.553 1.00 44.25
<b>ATOM</b>	2905 O	нон	93	36.591 7.772 23.374 1.00 68.23
<b>ATOM</b>	2908 O	HOH	94	34.274 5.197 22.878 1.00 51.62
<b>ATOM</b>	2911 O	HOH	95	41.935 7.033 29.073 1.00 63.23
<b>ATOM</b>	2914 O	HOH	96	20.731 12.105 14.716 1.00 54.80
<b>ATOM</b>	2917 O	НОН	97	23.147 13.682 17.882 1.00 50.81
<b>ATOM</b>	2920 O	нон	98	35.515 9.509 -3.558 1.00 56.70
<b>ATOM</b>	2923 O	HOH	99	38.933 9.503 -1.231 1.00 32.18
<b>ATOM</b>	2926 O	НОН	100	51.814 24.438 3.703 1.00 52.00
<b>ATOM</b>	2929 O	НОН	101	51.670 28.690 0.838 1.00 42.41
<b>ATOM</b>	2932 O	нон	102	46.536 30.610 1.750 1.00 45.80
<b>ATOM</b>	2935 O	HOH	103	45.165 34.214 0.818 1.00 46.46
<b>ATOM</b>	2938 O	нон	104	42.695 35.194 1.055 1.00 25.82
<b>ATOM</b>	2941 O	нон	105	39.689 33.418 0.723 1.00 31.99
ATOM	2944 O	нон	106	23.962 38.119 27.549 1.00 47.89
ATOM	2947 O	нон	107	25.343 40.908 27.379 1.00 54.09
ATOM		НОН	108	20.307 35.738 19.866 1.00 32.61
ATOM		НОН	109	28.085 54.303 18.810 1.00 61.58

# FIG. 7(56)

ATOM	2956 O	нон	110	29.849	56.131	16.966	1.00 37.29
ATOM	2959 O	HOH	111	31.503	58.023	14.735	1.00 46.45
<b>ATOM</b>	2962 O	HOH	112	35.212	55.981	10.499	1.00 92.07
<b>ATOM</b>	2965 O	HOH	113	36.530	55.812		1.00 30.72
<b>ATOM</b>	2968 O	HOH	114	50.045	41.251		1.00 82.26
<b>ATOM</b>	2971 O	HOH	115	25.153	36.460		1.00 50.86
<b>ATOM</b>	2974 O	HOH	116	31.749	32.705		1.00 30.04
<b>ATOM</b>	2977 O	HOH	117	30.213	3.806		1.00 39.74
<b>ATOM</b>	2980 O	HOH	118	36.511	1.159		1.00 41.62
<b>ATOM</b>	2983 O	HOH	119	27.155	4.637		1.00 79.92
<b>ATOM</b>	2986 O	HOH	120	57.319	11.287		1.00 33.02
<b>ATOM</b>	2989 O	HOH	121	52.121	12.483		1,00 45.55
<b>ATOM</b>	2992 O	HOH	122	47.613			1.00 41.01
<b>ATOM</b>	2995 O	HOH	123	57.550			1.00 30.62
<b>ATOM</b>	2998 O	HOH	124	32.338			1.00 35.48
<b>ATOM</b>	3001 O	HOH	125	31.065	5.698		1.00 42.74
<b>ATOM</b>	3004 O	HOH	126	32.603			1.00 33.30
<b>ATOM</b>	3007 O	HOH	127	34.394			1.00 42.12
<b>ATOM</b>	<b>3010 O</b>	HOH	128	37.961			1.00 47.57
<b>ATOM</b>	3013 O	HOH	129	42.215			1.00 45.13
<b>ATOM</b>	3016 O	HOH	130	46.307			1.00 70.02
<b>ATOM</b>	3019 O	HOH	131	50.369			1.00 42.22
<b>ATOM</b>	3022 O	HOH	132	47.231		22.930	
<b>ATOM</b>	3025 O	HOH	133	45.362			1.00 48.06
<b>ATOM</b>	3028 O	HOH	134	27.005			1.00 49.65
<b>ATOM</b>	3031 O	HOH	135	45.726			1.00 45.31
<b>ATOM</b>	3034 O	HOH	136	46.998	11.755		1.00 37.38
<b>ATOM</b>	3037 O	HOH	137	39.706	37.699		1.00 40.71
<b>ATOM</b>	3040 O	НОН	138	18.768	48.678		3 1.00 74.62
<b>ATOM</b>	3043 O	HOH	139	43.641			2 1.00 44.64
<b>ATOM</b>	3046 O	HOH	140	32.593			1.00 43.95
<b>ATOM</b>	3049 O	HOH	141				1.00 45.86
<b>ATOM</b>	3052 O	нон	142				3 1.00 35.99
<b>ATOM</b>	3055 O	HOH	143				1.00 33.09
<b>ATOM</b>	3058 O	нон			55.803		1.00 58.70
<b>ATOM</b>	<b>3061 O</b>	нон	145		<b>52.57</b> 4		1.00 68.48
<b>ATOM</b>					5 54.455		1.00 48.85
<b>ATOM</b>	<b>3067 O</b>	нон	147		40.725		1.00 62.58
<b>ATOM</b>					3 43.988		1.00 41.59
<b>ATOM</b>	3073 O	нон	149	36.626	45.045	6.144	1.00 54.04

# FIG. 7(57)

ATOM	3076 O	HOH	150	19.458 36.977 14.386 1.00 56.50
ATOM	3079 O	НОН	151	19.502 40.993 17.850 1.00 43.35
<b>ATOM</b>	3082 O	HOH	152	39.793 38.257 27.760 1.00 63.31
ATOM	3085 O	HOH	153	40.730 53.944 20.682 1.00 49.91
ATOM	3088 O	HOH	154	45.371 49.402 5.710 1.00 41.53
ATOM	3091 O	HOH	155	49.114 26.038 11.482 1.00 34.43
<b>ATOM</b>	3094 O	HOH	156	54.085 28.403 10.828 1.00 28.60
<b>ATOM</b>	3097 O	HOH	157	18.729 14.990 12.752 1.00 44.66
<b>ATOM</b>	3100 O	HOH	158	27.500 2.046 10.138 1.00 47.88
<b>ATOM</b>	3103 O	HOH	159	23.505 7.763 16.082 1.00 45.49
<b>ATOM</b>	3106 O	HOH	160	38.101 22.326 23.406 1.00 43.42
<b>ATOM</b>	3109 O	HOH	161	36.788 33.961 0.261 1.00 59.95
<b>ATOM</b>	3112 O	HOH	162	19.380 27.777 6.595 1.00 56.29
<b>ATOM</b>	3115 O	HOH	163	33.583 33.343 17.339 1.00 68.25
<b>ATOM</b>	3118 O	HOH	164	43.221 53.467 17.853 1.00 62.89
<b>ATOM</b>	3121 O	HOH	165	28.154 41.110 29.042 1.00 61.19
<b>ATOM</b>	3124 O	HOH	166	44.877 47.914 12.583 1.00 21.27
<b>ATOM</b>	3127 O	HOH	167	46.589 45.908 14.329 1.00 39.48
<b>ATOM</b>	3130 O	HOH	168	48.235 43.490 14.297 1.00 46.88
<b>ATOM</b>	3133 O	HOH	169	47.834 0.528 14.762 1.00 74.55
<b>ATOM</b>	3136 O	HOH	170	48.711 -2.009 16.386 1.00 52.45
<b>ATOM</b>	3139 O	HOH	171 .	41.210 0.396 17.381 1.00 58.05
<b>ATOM</b>	3142 O	HOH	172	43.837 1.538 17.483 1.00 72.30
<b>ATOM</b>	3145 O	HOH	173	41.780 -2.478 14.396 1.00 47.15
<b>ATOM</b>	3148 O	HOH	174	31.466 11.699 21.418 1.00 45.99
<b>ATOM</b>	3151 O	НОН	175	35.046 14.218 20.429 1.00 39.37
<b>ATOM</b>	3154 0	НОН	176	22.639 26.143 4.324 1.00 36.80
<b>ATOM</b>	3157 O	НОН		26.114 24.452 6.028 1.00 31.04
ATOM				28.927 30.687 4.252 1.00 41.38
ATOM	3163 O			23.899 6.610 18.621 1.00 56.43
ATOM				53.386 11.969 4.493 1.00 39.86
ATOM				30.051 43.727 0.910 1.00 47.97
<b>ATOM</b>	3172 O	НОН	182	31.659 49.099 8.149 1.00 52.84